NERL/ERD Publications

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Jan 1, 2003 - Dec 31, 2003 ***Presented Published***

ABSTRCT/ORAL

Russo, R.C., and Carousel, R.F. Louisiana environmental modeling system for hypoxia related issues. Presented at: Seventh International Symposium on Fish Physiology, Toxicology, and Water Quality, Tallinn, Estonia, May 12-15, 2003. 5/12/2003

Contact: Rosemarie C. Russo

Abstract: An environmental assessment tool to evaluate the impacts of nonpoint source (NPS) pollutants discharged from Mississippi River basins into the Gulf of Mexico and to assess their effects on receiving water quality will be described. This system (Louisiana Environmental Modeling System (LEMS) will build upon a joint effort by the U.S. Navy and EPA called the Northern Gulf Littoral Initiative (NGLI). This LEMS modeling system will expand on the state-of-the-art monitoring and coastal forecasting system developed for the Northern Gulf of Mexico. The modeling domain will be moved to the western side of Louisiana to encompass the hypoxic zone and the near coastal region. The modeling system will be linked to form a comprehensive modeling system for evaluating NPS discharges. The project should provide a technology that does not currently exist for the hypoxic zone, that combines a three-media model with an advanced coastal hydrodynamic and water quality model. This model to evaluate NPS discharges is important because of the impact on water quality including the formation of a hypoxic (dead) zone off the Louisiana coast line. The models mentioned above will be refined and coupled to produce the LEMS system, then applied to assess the water quality effects associated with NPS discharges on a larger scale in the Louisiana coastal regions of the Gulf of Mexico. Coupling the three-media model with the coastal hydrodynamic and water quality model will provide an innovative and useful approach to evaluate the impact of NPS discharges as they are transported and transformed through land runoff, surface stream networks, groundwater pathways and coastal tidal processes. The modeling system will help in defining the magnitude of reduction in NPS discharges to the Gulf of Mexico required to obtain a long-term decrease in the extent of hypoxia formation in the Gulf of Mexico.

Bird, S.L. Using canines in source detection of indoor air pollutants. Presented at: Indoor Air Quality Problems and Engineering Solutions Symposium, Research Triangle Park, NC, July 21-23, 2003. 7/21/2003

Contact: Sandra L. Bird

Abstract: Dogs have been used extensively in law enforcement and military applications to detect narcotics and explosives for over thirty years. Dogs are regularly used in arson investigations to detect accelerants since they are much more accurate at discriminating between accelerants and by-products of combustion than field VOC detectors. Controlled laboratory studies have documented accurate detection by dogs of specific compounds associated with explosives and narcotics at air concentrations below 1 ppb. Relatively few applications have taken advantage of this canine capability in the environmental arena. Dogs could be used to rapidly screen houses for problems such as vapor intrusion of a variety of VOCs, identifying the presence of mildews and toxic molds, or rapidly identifying houses where illicit pesticide use has occurred. Dogs can serve as a rapid screen to indicate the presence of a substance in air in a house and are also capable of moving towards the source of volatile materials. Benzene, toluene, ethylene, and xylene (BTEX) are major constituents of gasoline and frequent culprits in vapor intrusion into buildings from contaminated groundwater. Since indoor air contamination can also occur from household sources responsibility is often contested. This presentation demonstrates the use of dogs to signal the presence of the BTEX suite of compounds and the ability of the canines to move to the source of contamination.

Bird, S.L. Drift of pesticides: developing an integrated exposure tool. Presented at: Seminar at OPPTS, Washington, DC, June 18-19, 2003. 6/18/2003

Contact: Sandra L. Bird

Abstract: Off-site drift of pesticides from agricultural sites is a major source of inadvertant pesticide exposure. AgDRIFT/AGDISP is a near-field modeling technology (<1000 m) used to evaluate primary drift from a single application from a single field during neutral atmospheric conditions over level terrain with uniform surface characteristics. This technology is a major improvement for OPP in estimating exposure and gives them the ability to evaluate buffer zones, a range of application variables, and some environmental conditions. However, as it stands now many limitations exist in meeting OPP's total exposure assessment needs for pesticide drift. A new ORD research initiative is designed to develop and test modeling capabilities that will provide OPP, Regions, States, and other entities with the capability of addressing exposure from off-site drift in a comprehensive manner with quantifiable uncertainty. This seminar describes the current state of regulatory spray drift modeling technology and the current and proposed research efforts to develop a comprehensive tool.

Bird, S.L. Using canines in source detection of indoor air pollutants. Presented at: Indoor Air Quality Problems and Engineering Solutions Symposium, Research Triangle Park, NC, July 21-23, 2003. 7/22/2003

Contact: Sandra L. Bird

Abstract:

Burke, Jr., R.A., and Molinero, J. Trace gas concentrations in small streams of the Georgia Piedmont. Presented at: Georgia Water Resources Conference, Athens, GA, April 23-24, 2003. 4/23/2003

Contact: Roger A. Burke

Abstract: Seventeen headwater watersheds within the SFBR watershed ranging from 0.5 to 3.4 km2 were selected. We have been monitoring concentrations of the trace gases nitrous oxide, methane, and carbon dioxide, and other parameters (T, conductivity, dissolved oxygen, pH, nutrients, flow rate) on an approximately monthly basis for the last year. Percentages of forested land, agricultural and pasture land, residential areas, wetlands and open water surfaces within the watershed were calculated from the National Land Cover Data (NLCD) database. Nitrous oxide concentrations have varied widely from 10 nM (atmospheric equilibrium concentration) to nearly 80 nM among the streams. Overall, the streams draining watersheds dominated by developed land use have the highest dissolved nitrous oxide concentrations although the difference is statistically significant only for comparisons with the forest and mixed land use watersheds. Also, the streams draining watershed dominated by pasture have significantly greater nitrous oxide concentrations overall than streams draining forested watersheds. These results suggest that small streams could be a significant source of nitrous oxide to the atmosphere in some watersheds. Carbon dioxide concentrations in the stream range from about 30 to 900 microM (about 3 to 75 supersaturated with respect to the atmosphere). As for nitrous oxide, the streams draining residential areas had the highest overall carbon dioxide concentrations, although the only statistically significant comparison was with streams draining forested areas. Methane concentrations range from about 0.06 to 40 microM (about 30 to 20,000 supersaturated with respect to the atmosphere). Overall, streams draining watersheds dominated by pastures had significantly higher methane concentrations than streams draining any other land use type. As for nitrous oxide and carbon dioxide, the streams from forested watersheds had the lowest methane concentrations.

Molinero, J., and Burke, Jr., R.A. Relations between land use and stream nutrient concentrations for small watersheds in the Georgia Piedmont. Presented at: Georgia Water Resources Conference, Athens, GA, April 23-24, 2003. 4/23/2003

Contact: Roger A. Burke

Abstract: We have been sampling nutrient concentrations in 17 headwater streams within the South Fork Broad River (SFBR) watershed on a monthly basis since November 2001. The streams were classified as either developed (n=4), agriculture/pasture (n=4), mixed land use (n=6) or forested (n=3) based on information from the National Land Cover Data (NLCD) database. The lowest mean nitrogen concentrations were observed in streams draining forested watersheds. A set of landscape indicators explained 93 % of the spatial variability in the total nitrogen concentrations which suggests that watershed land use has an important effect on stream nitrogen levels. Total phosphorus varied seasonally at some of the sites, with high concentrations observed during the summer and low concentrations in winter. Only 4 out of 14 non-forested sites showed higher mean total phosphorus concentrations and no relationships were found between the landscape indicators and the total phosphorus concentrations in the streams. We suggest that, in contrast to what was observed for nitrogen, in-stream sources (e. g. decaying plant material), in-stream cycling, or strong pollution sources (e. g. manure, septic tanks) are more important than watershed land use in determining the total phosphorus concentrations in these small streams.

Molinero, J., and Burke, Jr., R.A. Dissolved organic carbon (DOC) concentrations in small streams of the Georgia Piedmont. Presented at: North American Benthological Society Annual Meeting, Athens, GA, May 27-31, 2003. 5/27/2003

Contact: Roger A. Burke

Abstract: Dissolved organic matter (DOM) supports microbial activity and contributes to transport of N and P in streams. We have studied the impact of land uses on dissolved organic carbon (DOC) concentrations in 17 Georgia Piedmont headwater streams since January 2001. We classified the watersheds as developed (n =4), pasture/agricultural (n=4), forested (n=3) and mixed land uses (n=6). Mean DOC concentrations were low (0.95-1.28 mg C/l) in forest streams and somewhat higher in other watersheds. However, no significant correlations were found between stream DOC and watershed land use, and neither population density, road density nor discharge explained a significant portion of DOC variability. A significant inverse correlation was found between DOC and oxygen concentrations (R2 = 0.70). DON was a variable portion (5 to 46 %) of the total dissolved nitrogen in the streams. We conclude that (1) conversion of forest to other land uses increases DOC in Georgia Piedmont streams, that (2) DOM influences dissolved oxygen concentrations and (3) plays a significant role in the transport of nitrogen in these streams, but (4) land use and several common landscape indicators are poor predictors of DOC concentrations.

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Presented Published

Burke, Jr., R.A. Trace gas concentrations in streams - early warning indicators of stream impairment?. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

Contact: Roger A. Burke

Abstract: Surface water contamination and resultant impairment of aquatic ecosystem functioning are serious environmental problems, caused in large part by land use changes and excess organic waste inputs associated with agriculture and residential and industrial development. Headwater streams are critical components of river networks, comprising ~95% of the total number of stream channels and ~75% of the total stream channel length in the US, and they frequently exhibit high rates of biogeochemical cycling. Because of their small size, headwater stream ecosystem function is easily impaired by human disturbance of the watershed, riparian zone, or channel. Headwater streams and their watersheds provide valuable ecosystem services such as organic matter processing which provides important resources to downstream ecosystems such as lakes and rivers. As watersheds are increasingly developed to meet human demands, the development of effective and easily measured indicators of watershed impairment will become increasingly crucial. The degrees to which stream concentrations of the biologically reactive trace gases nitrous oxide, carbon dioxide, and methane deviate from atmospheric equilibrium are useful indicators of overall watershed organic matter decomposition rates and metabolism (e.g., anoxic vs anaerobic, nitrification vs. denitrification). Because stream ecosystem function can be impaired by excess inputs of organic wastes, trace gas concentrations should provide valuable information about stream ecosystem function. Discussion of the need for effective indicators of organic waste and nutrient loadings to watersheds impacted by human activities with Region 4 and Office of Water (OW) personnel stimulated development of this research activity and it is anticipated that further development of these indicators will be made in collaboration with personnel from OW and various EPA Regions. Results of a one-year study of 17 Georgia Piedmont headwater streams suggest that: (1) total dissolved nitrogen (TDN), dissolved organic carbon (DOC), and dissolved concentrations of nitrous oxide and methane in streams are all effective indicators of stream impairment by nutrients and organic wastes from septic tanks and/or animal manure; and (2) the trace gas concentrations are far more sensitive indicators that respond to much lower levels of nutrient and organic waste contamination than do the bulk parameters TDN and DOC. Elevated levels of nitrous oxide and methane in streams appear to be viable early warning indicators of incipient stream impairment and these indicators, largely being developed through this research, may have great value to water quality managers and regulators in EPA Program Offices and Regions as well as those in state and local governments.

Burke, Jr., R.A., and Molinero, J. Trace gas concentrations in streams - early warning indicators of stream impairment?. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

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Burke, Jr., R.A., and Molinero, J. Trace gas and nutrient concentrations in small streams of the Georgia Piedmont. Presented at: Invited Seminar at the Joseph W. Jones Ecological Research Center, Newton, GA, August 21, 2003. 8/21/2003

Contact: Roger A. Burke

Abstract:

Carousel, R.F., and Russo, R.C. Louisiana environmental modeling system for hypoxia related issues. Presented at: Seventh International Symposium on Fish Physiology, Toxicology and Water Quality, Tallinn, Estonia, May 12-15, 2003. 5/12/2003

Contact: Robert F. Carousel

Abstract:

Garrison, A.W., Jones, W.J., Wiese, T.E., Washington, J.W., Jarman, J.L., and Avants, J. Observations of enantioselectivity in the fate, persistence and effects of modern pesticides. Presented at: 23rd International Symposium on Halogenated Organic Pollutants and Persistent Organic Pollutants, Boston, MA, August 24-29, 2003. 8/25/2003

Contact: Arthur W. Garrison

Abstract: Chiral pollutants exist as 2 (or more) species, -- enantiomers -- that are non-superimposable mirror images of each other. Enantiomers have identical physical and chemical properties except when they interact with enzymes or other chiral molecules; then they usually react selectively. This enantioselectivity often results in different rates of microbial/biological transformation, differences in toxicity of the two enantiomers, and differences in activities toward target species. Up to 25% of pesticides are chiral molecules, and almost all are manufactured and applied as their racemates, mixtures of equal amounts of the enantiomers. Recently, however, the agrochemical industry and government regulators are beginning to take enantioselectivity into account. For example, the (R)-(+)-enantiomer of dichlorprop (as well as the (R)-enantiomers of all the phenoxypropionic acid herbicides) is the herbicidally active species, while the (S)-(-)-enantiomer is inactive; so, to reduce the amount of herbicide used and avoid the possibility of the unnecessary enantiomer causing some adverse impact, several European countries have decreed that only the (R)-enantiomers will be used. In addition, the two (S)-enantiomers of metolachlor, one of the most widely used herbicides in the USA, are nine times more herbicidally active than the (R)-enantiomers, so its manufacturer successfully petitioned the EPA for registration of a formulation enriched to contain 88% of the (S)-enantiomers . This allows a 35% reduction in the amount of the herbicide applied, with the same effect. It seems obvious that the enantiomers of chiral pesticides should be treated as separate compounds and that accurate environmental and human risk assessments require an understanding of the relative persistence and effects of each enantiomer. This paper emphasizes results of recent research on the fate and effects of enantiomers of specific chiral pesticides in use today; the so-called modern pesticides.

Ulrich, E.M., Wong, C.S., Rounds, S.A., VanMetre, P.C., Wilson, J.T., Garrison, A.W., and Foreman, W.T. Enantiomer fractions of chlordane compounds in sediment samples from U.S. Geological Survey sites in lakes, rivers, and reservoirs. Presented at: Dioxin '03, Boston, MA, August 24-29, 2003. 8/25/2003

Contact: Arthur W. Garrison

Abstract: More than 500 important environmental contaminants are chiral (having structures that are nonsuperimposible mirror images). Although enantiomer pairs have identical physical-chemical properties, their toxicity, biodegradation, and environmental fate often are different. Cyclodextrin gas chromatography combined with mass spectrometry was used to determine the chiral characteristics of chlordane components in sediment. Enantiomer fractions [EF = area (+) enantiomer / sum of (+) and (-) areas] were used to determine if biological degradation had occurred in surficial and suspended-sediment samples, and if there was a trend with depth in sediment cores. Suspended sediment samples showed slight deviation from the racemic EF value of 0.50, suggesting that some biological degradation had occurred prior to sediment deposition in the water body. Surficial sediment samples also contained evidence of biodegradation [cis-chlordane (CC) = 0.492 - 0.620; trans-chlordane (TC) = 0.473 - 0.531; exo-heptachlor epoxide (HEPX) = 0.600 - 0.682]. At five core sites, EFs were close to racemic for TC and CC and in general, TC EFs were less than 0.5 and tend to increase slightly with depth, while the opposite was true for CC. There were no detectable amounts of two chlordane degradation products in sediment core samples. These results suggest that little biodegradation has occurred in the sediment core, and that historical concentration profiles should be unaltered by biological degradation processes. This work has been funded by the US EPA and USGS. It has been subjected to EPA review and approved for presentation. Mention of trade names of commercial products does not constitute endorsement or recommendation for use.

Ulrich, E.M., Wong, C.S., Rounds, S.A., VanMetre, P.C., Wilson, J.T., Garrison, A.W., and Foreman, W.T. Enantiomer fractions of chlordane compounds in sediment samples from U.S. Geological Survey sites in lakes, rivers and reservoirs. Presented at: 23rd International Symposium on Halogenated Organic Pollutants and Persistent Organic Pollutants, Boston, MA, August 24-29, 2003. 8/24/2003

Contact: Arthur W. Garrison

Abstract: The environmental behavior of the enantiomers of cis- and trans-chlordane has been the topic of much research since the first chiral separations on cyclodextrin gas chromatography (GC) columns. When chlordane is manufactured, it is always a racemic mixture (equal portion of two enantiomers). As the compounds move through the environment, physical processes, such as volatilization, photolysis, and OH radical reactions, are not likely to change the enantiomer signature. However, biological processes, including uptake, depuration, and metabolism often are mediated by chiral molecules, such as enzymes that cause changes in the enantiomer signature. Enantiomer behavior of chlordane has been reported in biota, soil, water, and air. Enantiomer signatures have been used to trace chlordane sources from soil in the Midwest, to air above the soil, and to air near the Great Lakes. Additionally, evidence of biological degradation has been shown through enantiomer signatures. To date there have been no reports of chlordane enantiomer trends in sediment. Previous studies of toxaphene congeners and PCB atropisomers in sediment samples have shown interesting enantioselective behavior. Because sediment cores are used as a historical record of contaminant deposition, it is important to ensure that the record is accurate and has not been changed by biological degradation. The goal of this research is to document the enantiomeric behavior of chlordane compounds in sediment samples. In addition to sediment cores, surficial and suspended sediment samples will help determine a likely source of contamination to sediment. Trends are analyzed with sediment type, location, deposition date, and concentration for various chlordane compounds.

Garrison, A.W., Jones, W.J., Wiese, T.E., Washington, J.W., Jarman, J.L., and Avants, J. Observations of enantioselectivity in the fate, persistence and effects of modern pesticides. Presented at: 23rd International Symposium on Halogenated Organic Pollutants and Persistent Organic Pollutants, Boston, MA, August 24-29, 2003. 8/25/2003

Contact: Arthur W. Garrison

Abstract:

Laniak, G.F. Overview of 3MRA technical approach. Presented at: Science Advisory Board Review, Washington, DC, August 26, 2003. 8/26/2003

Contact: Gerard F. Laniak

Abstract:

Laniak, G.F. Integrating the science and technology of environmental assessment across Federal Agencies. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

Contact: Gerard F. Laniak

Abstract: Seven Federal Agencies are conducting collaborative research to provide the next generation of environmental models for analyzing complex multimedia, multi-stressor contamination problems. Among the primary objectives of the Memorandum of Understanding (MOU) are 1) to provide a mechanism for the cooperating Federal Agencies to pursue a common technology in multimedia environmental modeling with a shared scientific basis, 2) to reduce redundancies and improve the common technology through exchange and comparisons of multimedia environmental models, software and related databases, 3) to exchange information related to multimedia environmental modeling tools and supporting scientific information for environmental risk assessments, protocols for establishing linkages between disparate databases and models, and development and use of a common model-data framework, and 4) to facilitate the establishment of working partnerships among the cooperating Federal Agencies' technical staff in order to enhance productivity and mutual benefit through collaboration on mutually-defined research studies. The collaborating agencies are (in addition to EPA/ORD):1. The United States Nuclear Regulatory Commission, Office of Nuclear Regulatory Research2. The United States Army Corps of Engineers, Engineer Research and Development Center3. The United States Department of Energy, Office of Science and Technology4. The United States Department of Interior, U.S. Geological Survey 5. The United States Department of Agriculture, Agricultural Research Service 6. The United States Department of Agriculture, Natural Resources Conservation Service The MOU is organized with a Steering Committee and several technical workgroups. The Steering Committee includes senior officials from each Agency and the workgroups are comprised of researchers from each Agency. To date workgroups have developed research plans (approved by the Steering Committee), sponsored sessions at professional conferences, and conducted workshops targeting details of potential collaborative projects. The current workgroups include :1. Software System Design and Implementation for Environmental Modeling2. Uncertainty Analysis and Parameter Estimation3. Distributive Watershed / Water Quality Modeling4. Reactive Solute Transport

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Contact: Gerard F. Laniak

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Laniak, G.F. The related role of environmental modeling frameworks. Presented at: International Workshop on Uncertainty, Sensitivity, and Parameter Estimation for Multimedia Environmental Modeling, Rockville, MD, August 19-21, 2003. 8/19/2003

Contact: Gerard F. Laniak

Abstract: In recent years the assessment of environmental systems for the purpose of regulatory decision making has expanded considerably from a medium-specific focus to a comprehensive assessment of contaminant movement from a source, through a multi-media environment (fate and transport), to human and ecological endpoints of concern. The key word with respect to this movement is integration. In the modeling community this means that groundwater modelers, atmospheric modelers, watershed modelers, surface water modelers, ecosystem modelers, and human and ecological exposure and risk modelers must now integrate their knowledge/models to formulate solutions that address all potential impacts. Conceptually, this is a rather straight forward undertaking. Practically, it is wrought with enormous challenges; most notably: 1) the access to, collection of, and organization of the wide array of required input data; 2) the specification of data flow among the science-based models in the system; and 3) the access to modeling tools needed for managing the model interactions, viewing/processing outputs, and assessing uncertainties and sensitivities. The objective of this presentation is to first describe the essential features of modern modeling frameworks, and, secondly, the benefits and challenges associated with integrating our collective framework development efforts in order to develop generic components that are interoperable, that is, components that will operate equally well in all frameworks. A primary conclusion offered in this presentation is the need to encourage developers of uncertainty and sensitivity methods, and models, to develop these tools in a framework independent manner.

Laniak, G.F. The related role of environmental modeling systems. Presented at: International Workshop on Uncertainty, Sensitivity, and Parameter Estimation for Multimedia Environmental Modeling, Rockville, MD, August 19-21, 2003. 8/21/2003

Contact: Gerard F. Laniak

Abstract:

Laniak, G.F. 3MRA Quality Assurance. Presented at: Science Advisory Board Review, Washington, DC, August 26, 2003. 8/21/2003

Contact: Gerard F. Laniak

Abstract:

Loux, N.T. DIFMOD2: A next generation diffuse layer model. Presented at: 39th International Union of Pure and Applied Chemistry Congress and 86th Conference of the Canadian Society for Chemistry, Ottawa, Canada, August 10-15, 2003. 8/10/2003

Contact: Nicholas T. Loux

Abstract: Jenne (1998) suggested that the majority of uncertainty in our current ability to model the environmental partitioning behavior of ionic species on natural surfaces resulted from uncertainties in our understanding of surface acidity behavior. Traditional 2-pK Grahame-Gouy-Chapman diffuse layer models of bound surface site acidity (>SOHx(x-1)) use mass action expressions of the following form: K = [>SOH(x-1)(x-2)]aH+EXP(- delta G (excess)/RT)/[>SOHx(x-1)] where EXP() is the exponential function, delta G (excess) = F psi (F = Faraday's constant and psi = surface potential) and the other symbols have their usual meaning. Recent findings suggest that this expression for delta G(excess) may be too simplistic. DIFMOD2, a next generation diffuse layer model, relies on a redefinition of delta G(excess): delta G(excess) = delta G(electrostatic) + delta G(hydration) + delta G(dipole) + delta G (act. coeff) + delta G(charging). The first four terms to the right of the equal sign have been discussed by Loux and Anderson, 2001 (Coll. Surfs. A., 177:123-131). Delta G(charging) is described by Loux (2000; Paper 114 of Env. Comp. And Geochem. Divisions, 219th ACS National Meeting) and Loux (2002; "Effective Acidity Constant Behavior Near Zero Charge Conditions", In Keane, M (Ed.), Interfacial Applications in Environmental Engineering, 2002). Although DIFMOD2 was developed using the Entropic Balanced Surface Potential Model (Loux, 1985; PhD thesis), a version based on traditional Poisson-Boltzmann theory will be introduced and used to explain anomalous effective acidity constant behavior near the pH (ZPC).

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Loux, N.T. Should latitudinal atmospheric trace vapor concentrations be reported on a mass density basis?. Presented at: Georgia Water Resources Conference, Athens, GA, April 23-24, 2003. 4/23/2003

Contact: Nicholas T. Loux

Abstract: For the past several decades the issue of global atmospheric trace vapor migration has been of concern to environmental professionals concerned with global distillation/cold condensation of toxic compounds, contamination of remote ecosystems, global climate change and stratospheric ozone depletion. In response to this concern, experimental databases of latitudinal trace vapor concentrations and global atmospheric transport models have been developed. These experimental databases typically contain vapor concentration data in units of mass concentration (e.g., ng/m3), volume fraction (e.g., parts per million) and mole fraction (e.g., parts per million). In contrast to measurements reported in units of volume and mole fractions, we will demonstrate that mass concentration data are functionally dependent on tropospheric temperature. Hence, the value of atmospheric trace gas concentration data reported on a mass concentration basis is severely limited unless concurrent atmospheric temperature, and perhaps even pressure and relative humidity data also are available.

Loux, N.T. DIFMOD2PB: A next generation diffuse layer model. Presented at: 39th International Union of Pure and Applied Chemistry Congress and 86th Conference of the Canadian Society for Chemistry, Ottawa, Ontario, August 10-15, 2003. 8/12/2003

Contact: Nicholas T. Loux

Abstract:

McCutcheon, S.C. Ecological engineering and phytoremediation: state of science and design. Presented at: Seminar at the University of Alabama, Birmingham, AL, August 28, 2003. 8/28/2003

Contact: Steven C. Mccutcheon

Abstract:

Smith, C.N., Spidle, D.L., Smith, P.D., Kitchens, B.E., Cyterski, M.J., Prieto, L.M., Bouchard, D.C., Wolfe, K., Kollig, H.P., Smith, L., Senter, S., Flexner, M., Cavinder, T.R., and Johnson, B. A comprehensive nonpoint source field study for sediment, nutrients and pathogens in the South Fork Broad River watershed, Georgia. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

Contact: Charles N. Smith

Abstract: There is an urgent need for EPA to develop protocols for establishing Total Maximum Daily Loads (TMDLs) in streams, lakes and estuaries. A cooperative TMDL field data collection project between ORD and Region 4 is ongoing in the South Fork Broad River Watershed (SFBR), a 245.18 square mile area with 337.32 stream miles located in the Savannah River Basin that consists of intensive storm event stream sampling. In 1998, the State of Georgia listed the SFBR watershed as biologically impaired (i.e. 303. (d) list), but the source of contamination was unknown. This project is 1) developing sampling protocols to measure the TMDL of bedload and suspended sediment, nutrients (nitrate, ammonia, ortho phosphorus and total phosphorus) total organic carbon and pathogens (fecal coliform, E. coli, and enterococci), and 2) developing a comprehensive database to develop, field test and apply mathematical models and protocols for calculating the TMDLs in this watershed and its tributaries in a field setting not available elsewhere in the U.S. Six stream sites have been highly instrumented with specialized monitoring equipment (ISCO water samplers, YSI multi-probes and cableway sampling systems) for collecting data before, during and after storm events. A weather station located in the watershed is collecting meteorological data and additional precipitation data are being collected from seven other sites. Stream hydrographic data are being collected for stage and velocity to develop stage-discharge relationships for each sampling site including a continuous real-time gaging station at the watershed outlet. When the study is complete, over three hundred stream cross-sectional sites will be surveyed and samples analyzed for characterization (particle size and carbon content by loss on ignition). Prior to the SFBR project, there was limited scientific data available to support TMDL development. The results of the SFBR project will accomplish the following: 1. Provide a comprehensive dataset that allows for the development, field testing, and calibration of mathematical models addressing water quality and quantity in a watershed. The dataset created in SFBR will be unique; there is no other study site with a comparable collection of data in the U.S. 2. Provide robust data and models that establish a scientific basis for clean sediment and pollutant TMDLs 3. Provide a means of testing field and laboratory instrumentation, methodolgy, and development of standard operating procedures for sampling protocols, sample processing and analytical analyses 4. Develop procedures for site selection, field instrumentation, maintenance and servicing, frequency of sampling, data requirements, safety and QA

Smith, C.N., Spidle, D.L., Stancil, F.E., Smith, P.D., Kitchens, B.E., Kollig, H.P., Smith, L., Senter, S., Cyterski, M.J., Prieto, L.M., Bouchard, D.C., Wolfe, K., Flexner, M., Cavinder, T.R., and Johnson, B. A comprehenisve nonpoint source field study for sediment, nutrients and pathogens in the South Fork Broad River Watershed in Northeast Georgia. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

Contact: Charles N. Smith

Abstract: There is an urgent need for EPA to develop protocols for establishing Total Maximum Daily Loads (TMDLs) in streams, lakes and estuaries. A cooperative TMDL field data collection project between ORD and Region 4 is ongoing in the South Fork Broad River Watershed (SFBR), a 245.18 square mile area with 337.32 stream miles located in the Savannah River Basin that consists of intensive storm event stream sampling. In 1998, the State of Georgia listed the SFBR watershed as biologically impaired (i.e. 303. (d) list), but the source of contamination was unknown. This project is 1) developing sampling protocols to measure the TMDL of bedload and suspended sediment, nutrients (nitrate, ammonia, ortho phosphorus and total phosphorus) total organic carbon and pathogens (fecal coliform, E. coli, and enterococci), and 2) developing a comprehensive database to develop, field test and apply mathematical models and protocols for calculating the TMDLs in this watershed and its tributaries in a field setting not available elsewhere in the U.S. Six stream sites have been highly instrumented with specialized monitoring equipment (ISCO water samplers, YSI multi-probes and cableway sampling systems) for collecting data before, during and after storm events. A weather station located in the watershed is collecting meteorological data and additional precipitation data are being collected from seven other sites. Stream hydrographic data are being collected for stage and velocity to develop stage-discharge relationships for each sampling site including a continuous real-time gaging station at the watershed outlet. When the study is complete, over three hundred stream cross-sectional sites will be surveyed and samples analyzed for characterization (particle size and carbon content by loss on ignition). Prior to the SFBR project, there was limited scientific data available to support TMDL development. The results of the SFBR project will accomplish the following:1. Provide a comprehensive dataset that allows for the development, field testing, and calibration of mathematical models addressing water quality and quantity in a watershed. The dataset created in SFBR will be unique; there is no other study site with a comparable collection of data in the U.S.2. Provide robust data and models that establish a scientific basis for clean sediment and pollutant TMDLs.3. Provide a means of testing field and laboratory instrumentation, methodolgy, and development of standard operating procedures for sampling protocols, sample processing and analytical analyses.4. Develop procedures for site selection, field instrumentation, maintenance and servicing, frequency of sampling, data requirements, safety and QA.

Weber, E.J., Collette, T.W., Jones, W.J., Kenneke, J.F., Mazur, C.S., Suarez, L.A., Stevens, C.T., Washington, J.W., Wolfe, K., Wolfe, N.L., Bailey, G.W., and Parmar, R.S. Modeling chemical fate and metabolism for computational toxicology. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

Contact: Eric J. Weber

Abstract: The goal of ORD's Computational Toxicology initiative is to develop the science for EPA to prioritize toxicity-testing requirements for chemicals subject to regulation. Many toxic effects, however, result from metabolism of parent chemicals to form metabolites that are much more toxic than the parent. Consequently, an accurate computerized simulator of metabolism is essential for meeting the objectives of the Computational Toxicology initiative. Because the liver is the primary organ for chemical metabolism, initial efforts will focus on the development of a metabolic simulator describing liver metabolism (i.e., a virtual liver). The primary goal of this research is to develop a computational system that will predict and prioritize metabolic pathways for the liver metabolism of organic chemicals.The metabolic simulator must allow for prioritization of many competing metabolic pathways for parent chemicals. The prioritization process requires the integration of reliable rate data. When this data is absent, it is necessary to populate a database with metabolic rate constants based on: 1) experimentally measured values, 2) rate constants derived from mechanistic-based SPARC or QSAR models, and 3) advanced spectroscopic techniques (e.g., NMR) for measuring metabolic rate constants and identifying metabolites in vivo and in vitro. An initial challenge of this research is the selection of representative chemicals for study. To ensure focus on the highest priority chemicals, a workgroup specifically on metabolism will be formed. Such a workgroup will allow partners outside of ORD (e.g., OPPT, OSW and OW) an opportunity to have their priority questions answered in addition to the ORD research agenda.

Weber, E.J., Parmar, R.S., Bailey, G.W., Collette, T.W., Hilal, S.H., Jones, W.J., Kenneke, J.F., Mazur, C.S., Suarez, L.A., Stevens, C.T., Washington, J.W., Wolfe, K., and Wolfe, N.L. Modeling chemical fate and metabolism for computational toxicology. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

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Zepp, R.G., Moran, M.A., and Koopmans, D. Photoreactivity of chromophoric dissolved organic matter (CDOM) derived from decomposition of various vascular plant and algal sources. Presented at: 225th American Chemical Society National Meeting, New Orleans, LA, March 23-27, 2003. 3/23/2003

Contact: Richard G. Zepp

Abstract: Chromophoric dissolved organic matter (CDOM) in aquatic environments is derived from the microbial decomposition of terrestrial and microbial organic matter. Here we present results of studies of the spectral properties and photoreactivity of the CDOM derived from several organic matter sources found in watersheds and coastal regions of the Southeastern United States. The species examined were derived from microbial decomposition of litter from two woody vascular plants (live oak, loblolly pine), two non-woody vascular plants (Spartina, the sea grass Thalassia) and the algal species Synechococcus. Absorption properties of the algal CDOM were significantly different that those of the CDOM derived from the terrestrial, vascular plant sources. For example, the spectral slope coefficient of the UV-visible spectra ranged from 0.028 nm(-1) for the Synechococcus CDOM to 0.010-0.015 nm(-1) for the vascular plant derived CDOM. Photoreaction of all the CDOM on exposure to simulated solar radiation resulted in increases in the spectral slope coefficients and blue shifts in their excitation-emission fluorescence spectra. The photodegradation rate constant of the Synechococcus CDOM, judged by its photobleaching at 350 nm, was almost an order of magnitude greater than that of the terrestrially derived CDOM. Exposure of CDOM from these sources produced measurable biologically labile photoproducts, even in extensively degraded material.

Xie, H., Zafiriou, O.C., Cai, W.J., and Zepp, R.G. Effects of sunlight on carboxyl content of dissolved organic matter in the Satilla River of Georgia, United States. Presented at: 225th American Chemical Society National Meeting, New Orleans, LA, March 23-27, 2003. 3/23/2003

Contact: Richard G. Zepp

Abstract: A study examined the effect of sunlight-initiated photo-degradation of dissolved organic matter (DOM) on its carboxyl content, and the role of oxygen and iron in this process. Solar-simulated irradiations were performed on 0.2-mm filtered water samples collected from the highly colored Satilla River in Georgia, USA. Prior to the irradiations the samples were purged with air, pure oxygen or pure nitrogen to obtain three different initial oxygen levels: air-, oxygen- or nitrogen-saturated, respectively. The influence of iron was studied by comparing samples with and without addition of deferrioxamine mesylate, a strong, photochemically inert, iron-complexing ligand. The carboxyl contents of DOM before and after irradiations were determined using potentiometric titrations. Photochemically induced loss of absorbance and dissolved organic carbon (DOC), production of carbon dioxide (CO_2), oxygen consumption, and variations of pH and [Fe(II)] were also monitored. For all the treatments, the carboxyl content in mmoles per liter of sample did not change significantly over the time course of irradiation up to 46 hours. However, the DOC-normalized carboxyl content (mmol/mg C) after 46 hour of exposure increased by a factor of 1.6 and 2.6 in the air- and oxygen-saturated samples, respectively. The variations of the DOC-normalized carboxyl content in all other treatments were within the experimental uncertainty. The results unequivocally indicate that the prolific photoproduction of CO_2, which has long been hypothesized as a result of photodecarboxylation of DOM, cannot be accounted for by the changes of carboxyl content observed. In addition, methylation of the carboxylic groups on DOM reduced the rate of CO_2 production only by 25%. This study, therefore, strongly suggests that the primary mechanism for photoproduction of CO_2 was not photodecarboxylation or that carboxylic groups were photochemically regenerated.

White, E.M., Vaughan, P.P., and Zepp, R.G. Photocheical production of hydroxyl radical in natural water - the role of iron and dissolved organic matter. Presented at: 225th American Chemical Society National Meeting, New Orleans, LA, March 23-27, 2003. 3/23/2003

Contact: Richard G. Zepp

Abstract: Photochemical hydroxyl radical (OH) production was measured in several natural waters to investigate the importance of colored dissolved organic matter (CDOM) and iron-CDOM complexes as sources of OH. High rates of OH photoproduction in highly colored, iron-rich, acidic waters are likely due to the involvement of photo-Fenton reactions, in which iron(II) and iron(II)-CDOM complexes react with hydrogen peroxide. The production of OH, hydrogen peroxide and iron(II) was monitored during the irradiation of Satilla River water, providing evidence of photo-Fenton produced OH. Addition of iron chelators, to inhibit the photoreduction of iron, reduced photochemical OH production, further indicating this pathway. The effects of OH on the optical properties of CDOM, through OH scavenging by CDOM, were also investigated for the Satilla River and other waters. Changes in the absorbance and fluorescence properties of these waters were observed in the presence of added OH sources and scavengers.

Zepp, R.G. Interactions of climate change and UV radiation as corals stressors. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/7/2003

Contact: Richard G. Zepp

Abstract:

Kisselle, K., Zepp, R.G., Molina, M., Burke, Jr., R.A., and Franzluebbers, A.J. Effects of fertilizer type (chicken litter vs. inorganic fertilizer) and cattle grazing on the soil microbial community. Presented at: 2003 Annual Symposium: Soil Biodiversity and Function, Lancaster, UK, March 25-27, 2003. 3/25/2003

Contact: Richard G. Zepp

Abstract: Pasture plots included unharvested, hayed, light and heavy cattle grazing pressure, fertilized with either inorganic N-P-K or broiler litter. Total phospholipid fatty acids (PLFAs) followed a seasonal trend and were higher in grazed plots than hayed & unharvested plots. Fungi and protozoa made up a larger percentage of the microbial community during the growing season, while bacteria and actinomycetes made up more in the autumn samples. Broiler litter plots had less fungi and slightly more bacteria and actinomycetes than plots receiving inorganic fertilizer. The hayed treatment had higher quantities of protozoan PLFAs and smaller quantities of bacterial PLFAs. Indirect evidence of top-down control of bacterial populations in all plots is given by a significant inverse relationship between a protozoan PLFA and the sum of several bacterial PLFAs.

Zepp, R.G. Shedding light on corals health: interactions of climate change and solar radiation with bleaching. Presented at: Corals Reefs, Climate, and Coral Bleaching Workshop, Oahu, HI, June 18-20, 2003. 6/18/2003

Contact: Richard G. Zepp

Abstract: Coral bleaching and declines in coral reef health in recent years have been attributed in part to processes driven by UV and/or visible light. For coral assemblages, exposure to UV light is often an unavoidable consequence of having access to visible (photosynthetically active) radiation. UV exposure can potentially affect corals by damage to DNA or by damage to other target molecules, including proteins that are part of the photosynthetic system. Changes in environmental conditions such as increased temperature or other factors can influence adverse responses of corals to UV and visible light by altering mechanisms that protect the corals from light damage. In addition to effects on responses of corals to UV light, changes in environmental conditions can also have pronounced effects on the nature and amount of light that reaches the surface of corals, especially in the UV region. Changes in atmospheric composition, especially in total ozone, have important effects on the UV-B (280 - 315 nm) part of solar radiation that reach the ocean surface. In addition, changes in UV exposure can stem from shifts in UV-absorbing dissolved and particulate organic matter in the ocean. Recent research has shown that the colored component of dissolved organic matter (CDOM) controls the penetration of solar UV and blue radiation into waters over the many coral reefs. Light exposure of the CDOM in the upper ocean causes it to decompose and the resulting decrease in UV light absorption can enhance UV exposure of coral reefs, especially under well-stratified conditions such as those that develop during El Nino events. The CDOM is introduced to the water by decomposition of aquatic plants (e.g. algal detritus and seagrasses) and by runoff from nearby terrestrial ecosystems. Changes in salinity and land use, coupled with precipitation, sea level and current changes, can have important effects on CDOM sources that affect corals light exposure.

Zhang, Z.Z., and Bailey, G.W. Modeling of metal binding on humic substances using the NIST database: an a priori functional group approach. Presented at: Seventh International Symposium on Fish Physiology, Toxicology, and Water Quality, Tallinn, Estonia, May 12-15, 2003. 5/12/2003

Contact: George W. Bailey

Abstract: Various modeling approaches have been developed for metal binding on humic substances. However, most of these models are still curve-fitting exercises-- the resulting set of parameters such as affinity constants (or the distribution of them) is found to depend on pH, ionic strength, and concentrations of metals and humic substances. Consequently, these models are not satisfactory to predict metal binding under environmental settings. We have developed an a priori model based on the elemental composition and functional group concentrations of humic substances, using the National Institute of Standard and Technology (NIST) database of critically selected stability constants of metal complexes. We tabulated the stability constants of metal complexes with selected functional groups and have plotted the corresponding conditional stability constants at several pH levels. These data showed that in addition to oxygen-bearing groups, the nitrogen-bearing groups and sulfur-bearing groups are also important for metal binding. The amino acid group plays a significant role for binding of Cu(II), Hg(II), Cr(III) and Fe(III), whereas the SH-functional group is important for the binding of soft Lewis acids' metals, such as Cd(II), Hg(II), and Pb(II). We have shown that such a simple model is capable of predicting adsorption and competitive adsorption of metals when the concentration of metals is below 10(-5) to 10(-6) M, which is the relevant metal concentration under most environmental settings.

Richardson, S.D., Thruston, Jr., A.D., Krasner, S.W., Weinberg, H.S., Chinn, R., Sclimenti, M.J., Pastor, S.J., and Onstad, G.D. Disinfection by-products of health concern in drinking water: results of a U.S. nationwide occurrence study. Presented at: International Mass Spectrometry Conference, Edinburgh, Scotland, August 31 - September 5, 2003. 8/31/2003

Contact: Susan D. Richardson

Abstract: Drinking water disinfection by-products (DBPs) are of concern because some epidemiologic studies have shown that some DBPs are associated with cancer or adverse reproductive/developmental effects in human populations, and other studies have shown that certain DBPs cause similar health effects in laboratory animals. As a result, the U.S. Environmental Protection Agency (EPA) has regulated several DBPs; however, most DBPs have not been tested for adverse health effects due to the high costs involved. In order to prioritize new DBPs for health effects testing, we initiated a Nationwide Occurrence Study to quantify 'high priority' DBPs (those predicted by toxicology experts to possibly have an adverse health effect) to determine how often they occur and at what levels. The fate and transport of these DBPs in the distribution system was also studied, and new DBPs were identified. Drinking water samples were collected across the United States from 12 plants that use chlorine, ozone, chlorine dioxide, and/or chloramines for disinfection. Locations were chosen to provide waters that contain low and high bromide levels, different pH conditions, and different natural organic matter (NOM) levels (NOM and bromide are DBP precursors; pH impacts the formation and stability of many DBPs). For comparison purposes, regulated and Information Collection Rule DBPs were quantified along with the high priority DBPs. Drinking water samples were collected at the treatment plants and in the distribution systems. Quantitation methods developed involved various extraction, derivatization, and detection methods (including solid-phase extraction, liquid-liquid extraction, solid-phase microextraction, and purge-and-trap with GC/electron capture detection or GC/MS). For identifying new DBPs, GC with low and high resolution electron ionization-MS and chemical ionization-MS were used.

Many of the high priority DBPs were found in drinking waters across the United States. High priority DBPs identified and quantified include 3-chloro-4-(dichloromethyl)-5-hydroxy-2(5H)-furanone (MX) and brominated forms of MX (the so-called BMXs), iodo-trihalomethanes, other halomethanes, halonitromethanes, haloacids, haloacetaldehydes, haloacetonitriles, haloketones, haloacetates, haloamides, and a few non-halogenated DBPs. In previous limited studies, MX was found at levels up to 60 parts-per-trillion (ng/L); however, in this study, MX reached levels of 300-400 ng/L at certain locations. Iodinated DBPs, including iodo-trihalomethanes, were also detected in many drinking waters sampled, even those with relatively low bromide (and probably low iodide) levels. Although chloramines are used to reduce trihalomethane formation, previous bench-scale studies indicated that ammonia addition before chlorination (to form chloramines) could favor the formation of iodinated DBPs. In this full-scale study, iodo-trihalomethanes were highest at a plant that used chloramines only for disinfection. Also while ozone and chloramines generally control the formation of trihalomethanes and other trihalo species, some dihalo species (such as dihaloaldehydes) were higher at plants using ozonation and/or chloramination. Another important finding was the discovery of iodo-acids. Iodo-acids have never been reported previously for any disinfectant. Five iodo-acids (iodoacetic acid, iodobromoacetic acid, iodobromopropenoic acid (2 isomers), and 2-iodo-3-methylbutenedioic acid) were identified in drinking water from a plant in the Southwest that used chloramine disinfection for high-bromide source waters. Many new brominated haloacids were also identified in drinking waters from several states. Brominated DBPs are important, as current toxicology (and some recent epidemiology) studies suggest that certain brominated DBPs may be of higher health concern than the chlorinated species.

Plewa, M.J., Wagner, E.D., Kim, A.C., Nelson, R., and Richardson, S.D. Mammalian cell cytotoxicity and genotoxicity of new drinking water disinfection by-products. Presented at: 2003 Environmental Mutagen Society Conference, Miami, FL, May 10-14, 2003. 5/10/2003

Contact: Susan D. Richardson

Abstract: The disinfection of drinking water continues to protect the public health against acute disease. Drinking water disinfection by-products (DBPs) are formed by the reaction of a disinfectant with naturally occurring organic matter. Many DBPs are genotoxic and are implicated as human carcinogens and teratogens. Two new DBPs, 2,3,5-tribromopyrrole (TBP) and iodoacetic acid (IA) were isolated and chemically characterized. TBP was isolated from chlorine dioxide-chlorine and chlorine dioxide-chloramine treated water from the Sea of Galilee, Israel, that contained bromide levels of approximately 2 mg/L. This is the first time a halopyrrole has been identified as a DBP. Using a microplate-based chronic cytotoxicity assay, TBP was a strong cytotoxin in Chinese hamster ovary (CHO) cells. The concentration of TBP that reduced the CHO cell density by 50% (%C?) after 72 h exposure was 60.6 microM. At concentrations above 150 microM, TBP induced genomic DNA damage in CHO cells treated for 4 h using the single cell gel electrophoresis (SCGE comet) assay. IA was identified in chloramine-treated drinking water from Texas, U.S.A. that contained bromide levels of 0.25 mg/L. IA is a very potent CHO cell chronic cytotoxin with a %C? value of 2.9 microM. IA is also the strongest genotoxic agent of the 22 DBPs we have analyzed. IA at concentrations of 5 microM and above after 4 h exposure induced genomic DNA damage in CHO cells. For the monohalogenated acetic acids the rank order, from high to low toxicity, for both CHO cell chronic cytotoxicity and acute genotoxicity was iodoacetic acid > bromoacetic acid >> chloroacetic acid.

Richardson, S.D., Thruston, Jr., A.D., Krasner, S.W., Weinberg, H.S., Chinn, R., Sclimenti, M.J., Pastor, S., and Onstad, G.D. Disinfection by-products of health concern in drinking water: results of a nationwide occurrence study. Presented at: 51st American Society for Mass Spectrometry Conference, Montreal, Canada, June 8-12, 2003. 6/8/2003

Contact: Susan D. Richardson

Abstract: Drinking water disinfection by-products (DBPs) are of concern because some epidemiologic studies have shown that some DBPs are associated with cancer or adverse reproductive/developmental effects in human populations, and other studies have shown that certain DBPs cause similar health effects in laboratory animals. As a result, the U.S. Environmental Protection Agency (EPA) has regulated several DBPs; however, most DBPs have not been tested for adverse health effects due to the high costs involved. In order to prioritize new DBPs for health effects testing, we initiated a Nationwide Occurrence Study to quantify 'high priority' DBPs (those predicted by toxicology experts to possibly have an adverse health effect) to determine how often they occur and at what levels. The fate and transport of these DBPs in the distribution system was also studied, and new DBPs were identified.

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Richardson, S.D. Disinfection by-products of health concern in drinking water: results of a nationwide occurrence study. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

Contact: Susan D. Richardson

Abstract: The Safe Drinking Water Act and Amendments requires that EPA address disinfection by-products (DBPs) in drinking water. DBPs are formed when a disinfectant (such as chlorine) reacts with organic matter and/or bromide naturally present in source waters. Drinking water disinfection by-products (DBPs) are of concern because epidemiologic studies indicate that some may be responsible for cancer and reproductive/developmental effects in human populations, and other studies have shown that certain DBPs cause cancer in laboratory animals. A few DBPs are regulated; however, most DBPs have not been tested for adverse health effects due to high costs involved. In order to prioritize new DBPs for health effects testing, we initiated a Nationwide Occurrence Study to quantify ?high priority' DBPs (those predicted by experts to potentially cause an adverse health effect at relatively low doses) to determine how often they occur and at what levels. The fate and transport of these DBPs in the distribution system was also studied, and new DBPs were identified. Scientists from the University of North Carolina and the Metropolitan Water District of Southern California collaborated with NERL scientists on this effort. Drinking waters were chosen across the United States in locations to provide waters with low and high bromide, different pH conditions, and different organic matter levels. Regulated and Information Collection Rule DBPs were also measured for comparison purposes. Analytical methods were developed for quantifying the high priority DBPs in drinking water, and mass spectrometry methods were used to identify new DBPs. Most of the high priority DBPs were found in drinking waters across the U.S.. High priority DBPs identified and quantified include 3-chloro-4-(dichloromethyl)-5-hydroxy-2(5H)-furanone (MX), brominated forms of MX, iodo-trihalomethanes, halomethanes, halonitromethanes, haloacids, haloacetonitriles, haloketones, haloacetates, haloamides, and a few non-halogenated DBPs. Significant results include finding MX at much higher levels than previously believed possible (300-400 ng/L), finding the highest levels of iodo-THMs at a plant using chloramines for disinfection, and finding the highest levels of dihaloaldehydes at a plant using ozonation. In addition, iodo-acids were identified for the first time as DBPs, as well as several new brominated haloacids. Brominated DBPs are important, as toxicology studies suggest that certain brominated DBPs may be of higher health concern than the chlorinated species.This research expands our knowledge on the occurrence of DBPs beyond those that are currently regulated, will help to prioritize future DBP health effects research, and will allow EPA's Office of Water to make improved decisions regarding the safety of drinking water and to ultimately minimize any that are found to be hazardous.

Richardson, S.D., Thruston, Jr., A.D., Krasner, S.W., Weinberg, H.S., Chinn, R., Sclimenti, M.J., Pastor, S.J., and Onstad, G.D. Emerging disinfection by-products of toxicological interest: results of a nationwide occurrence study. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

Contact: Susan D. Richardson

Abstract: The Safe Drinking Water Act and Amendments requires that EPA address disinfection by-products (DBPs) in drinking water. DBPs are formed when a disinfectant (such as chlorine) reacts with organic matter and/or bromide naturally present in source waters. Drinking water disinfection by-products (DBPs) are of concern because epidemiologic studies indicate that some may be responsible for cancer and reproductive/developmental effects in human populations, and other studies have shown that certain DBPs cause cancer in laboratory animals. A few DBPs are regulated; however, most DBPs have not been tested for adverse health effects due to high costs involved. In order to prioritize new DBPs for health effects testing, we initiated a Nationwide Occurrence Study to quantify ?high priority' DBPs (those predicted by experts to potentially cause an adverse health effect at relatively low doses) to determine how often they occur and at what levels. The fate and transport of these DBPs in the distribution system was also studied, and new DBPs were identified. Scientists from the University of North Carolina and the Metropolitan Water District of Southern California collaborated with NERL scientists on this effort. Drinking waters were chosen across the United States in locations to provide waters with low and high bromide, different pH conditions, and different organic matter levels. Regulated and Information Collection Rule DBPs were also measured for comparison purposes. Analytical methods were developed for quantifying the high priority DBPs in drinking water, and mass spectrometry methods were used to identify new DBPs. Most of the high priority DBPs were found in drinking waters across the U.S.. High priority DBPs identified and quantifiedinclude 3-chloro-4-(dichloromethyl)-5-hydroxy-2(5H)-furanone (MX), brominated forms of MX, iodo-trihalomethanes, halomethanes, halonitromethanes, haloacids, haloacetonitriles, haloketones, haloacetates, haloamides, and a few non-halogenated DBPs. Significant results include finding MX at much higher levels than previously believed possible (300-400 ng/L), finding the highest levels of iodo-THMs at a plant using chloramines for disinfection, and finding the highest levels of dihaloaldehydes at a plant using ozonation. In addition, iodo-acids were identified for the first time as DBPs, as well as several new brominated haloacids. Brominated DBPs are important, as toxicology studies suggest that certain brominated DBPs may be of higher health concern than the chlorinated species. This research expands our knowledge on the occurrence of DBPs beyond those that are currently regulated, will help to prioritize future DBP health effects research, and will allow EPA's Office of Water to make improved decisions regarding the safety of drinking water and to ultimately minimize any that are found to be hazardous.

Richardson, S.D. Do you know what's in your drinking water? Identifying the chemical by-products you can't see. Presented at: Northeast Georgia Engineers Meeting, Athens, GA, June 20, 2003. 6/20/2003

Contact: Susan D. Richardson

Abstract:

Richardson, S.D., Thruston, Jr., A.D., Krasner, S.W., Weinberg, H.S., Chinn, R., Sclimenti, M.J., Pastor, S.J., and Onstad, G.D. Disinfection by-products of health concern in drinking water: results of a nationwide occurrence study. Presented at: 51st American Society for Mass Spectrometry Conference, Montreal, Canada, June 8-12, 2003. 6/8/2003

Contact: Susan D. Richardson

Abstract:

Thruston, Jr., A.D., Richardson, S.D., Couillard, L.A., Lewis, C., and Klappa, P. GC/MS identification of drinking water disinfection by-products from Milwaukee's new ozonation plants. Presented at: 51st American Society for Mass Spectrometry Conference, Montreal, Canada, June 8-12, 2003. 6/8/2003

Contact: Alfred D. Thruston

Abstract: The Milwaukee Water Works recently added ozonation disinfection facilities to their municipal drinking water treatment. Coupling ozone treatment with biologically active filtration (BAF) was seen as a logical step to enhance multiple water quality objectives (an effective barrier to further Cryptosporidium contamination in light of the 1993 outbreak, in which 400,000 people became ill, and 100 people died), and fit current industry and regulatory trends toward organics removal. Because of concerns about potential increased levels of disinfection by-products (DBPs) in the finished water resulting from ozonation, special emphasis was placed on the use of biological filtration as a technique to potentially remove most of these DBPs from the finished water - which is of growing interest in the U.S. This led to a collaboration with EPA's National Exposure Research Laboratory (NERL) facility in Athens, GA to collect a series of samples from various stages of water treatment from the Milwaukee plant in August 2002. These samples were analyzed for a comprehensive list of DBPs (including many DBPs that are not regulated).

Thruston, Jr., A.D., Richardson, S.D., Couillard, L.A., Lewis, C., and Klappa, P. GC/MS identification of drinking water disinfection by-products from Milwaukee's new ozonation plants. Presented at: 51st American Society for Mass Spectrometry Conference, Montreal, Canada, June 8-12, 2003. 6/8/2003

Contact: Alfred D. Thruston

Abstract:

Jones, W.J., O'Niell, W.L., Mazur, C.S., Kenneke, J.F., and Garrison, A.W. Enantioselective transformation of chiral PCBs and fipronil in anoxic sediments. Presented at: 23rd International Symposium on Halogenated Organic Pollutants and Persistent Organic Pollutants, Boston, MA, August 24-29, 2003. 8/26/2003

Contact: William J. Jones

Abstract:

Frick, W.E. Predicting bacterial concentration on the nation's beaches. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

Contact: Walter E. Frick

Abstract: A classical example of the failure of institutions and environmental technology to protect the nation's aesthetic, recreational, and public health values is represented by the July-August, 1999 Huntington Beach, California beach closure. This multi-million dollar regional public health disaster (high bacterial concentrations) affected perhaps a million vacationers and may be compared with major environmental disasters, such as the Exxon Valdez oil spill, in shaping public perceptions. The short-term result was the abandonment, under intense political pressure, of the local sanitation district's 301(h) waiver of secondary treatment privileges. As an important discharger in the area, it has committed to upgrade to full secondary treatment and to chlorine disinfection of the effluent discharged more than four miles offshore, at a capital improvement cost estimated to range from $250M to $400M.However, an independent science review of extensive monitoring data has yet find a strong link between offshore plume concentrations and distribution and surf zone elevated bacterial levels, the two regions being separated by bands of much lower concentrations. There are indications that other sources ? a power plant's effluent also serving combined sewer overflows, the Santa Ana River, a bird sanctuary, public toilets, and unidentified renegade sources ? may be important determinants of surf zone pollution. Meanwhile, bacterial sampling typically requires 48-hour incubation times, severely decreasing the ability of bacterial monitoring programs to both protect public health and optimize public access to beaches. This project envisions the formulation of a model, working title Visual Beach, to be based on the EPA Visual Plumes program and other models and water circulation estimation techniques. In collaboration with the Orange County Sanitation District, it will be tested against routine monitoring conducted by the District. If successful, the model may help develop effluent disinfection that will prevent high waste-field concentration when shoreward movement is forecasted. Secondly, the model may help identify other potential sources contributing to the high bacterial levels, leading to their remediation. The ultimate product will utilize telemetered real-time monitoring data and fluid dynamical models and prognostic products to predict surf zone bacterial concentrations with enough lead time to allow for adequate disinfection of the district's effluent, identification of contributing sources, and health advisory lead times.

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Frick, W.E., and Molina, M. Predicting bacterial concentration on the Nation's beaches. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

Contact: Walter E. Frick

Abstract: A classical example of the failure of institutions and environmental technology to protect the nation's aesthetic, recreational, and public health values is represented by the July-August, 1999 Huntington Beach, California beach closure. This multi-million dollar regional public health disaster (high bacterial concentrations) affected perhaps a million vacationers and may be compared with major environmental disasters, such as the Exxon Valdez oil spill, in shaping public perceptions. The short-term result was the abandonment, under intense political pressure, of the local sanitation district's 301(h) waiver of secondary treatment privileges. As an important discharger in the area, it has committed to upgrade to full secondary treatment and to chlorine disinfection of the effluent discharged more than four miles offshore, at a capital improvement cost estimated to range from $250M to $400M.However, an independent science review of extensive monitoring data has yet find a strong link between offshore plume concentrations and distribution and surf zone elevated bacterial levels, the two regions being separated by bands of much lower concentrations. There are indications that other sources ? a power plant's effluent also serving combined sewer overflows, the Santa Ana River, a bird sanctuary, public toilets, and unidentified renegade sources ? may be important determinants of surf zone pollution. Meanwhile, bacterial sampling typically requires 48-hour incubation times, severely decreasing the ability of bacterial monitoring programs to both protect public health and optimize public access to beaches. This project envisions the formulation of a model, working title Visual Beach, to be based on the EPA Visual Plumes program and other models and water circulation estimation techniques. In collaboration with the Orange County Sanitation District, it will be tested against routine monitoring conducted by the District. If successful, the model may help develop effluent disinfection that will prevent high waste-field concentration when shoreward movement is forecasted. Secondly, the model may help identify other potential sources contributing to the high bacterial levels, leading to their remediation. The ultimate product will utilize telemetered real-time monitoring data and fluid dynamical models and prognostic products to predict surf zone bacterial concentrations with enough lead time to allow for adequate disinfection of the district's effluent, identification of contributing sources, and health advisory lead times.

Weaver, J.W. Software tools for assessment of contaminated sites. Presented at: U.S. EPA Office of Underground Storage Tanks Annual Conference, San Francisco, CA, March 10-12, 2003. 3/12/2003

Contact: James W. Weaver

Abstract: Models have become an integral part of decision-making for many LUST sites if only because they form the basis of RCBA tiered assessments. Models, though, are based on a series of assumptions concerning how chemicals behave in the environment, how water flows through the ground, even how a contaminant release occurs. How can you identify these assumptions? We'll present a field guide to models that helps identify model assumptions and their impacts on model results. Data is important too and we'll show how the amount and quality of available data affect model results. In practice, inputs to models are selected from various sources, including measurements, literature, defaults, estimates, and calibration. A number of these issues are addressed by a set of on-line calculators that EPA developed for assessment of contaminated sites. We'll look at calculators that can be used to estimate parameters, convert units, assess uncertainties in calculations. Participants that bring laptops can run the calculators themselves from a CD that will be provided. Lastly we'll look at ways to evaluate modeling work. Some steps of evaluation of models can be boiled down to nearly a recipe; also needed are knowledge of fate and transport, modeling in general, and the specific details of the model used.

Wang, Z., Hollebone, B., Fingas, M., Fieldhouse, B., Sigouin, L., Landriault, M., Noonan, J., and Weaver, J.W. Development of a composition database for selected multicomponent oils. Presented at: International Oil Spill Conference, Vancouver, Canada, April 7-10, 2003. 4/7/2003

Contact: James W. Weaver

Abstract: During any oil spill incident, the properties of the spilled oil, including its chemical composition, physical properties, and changes due to weathering, are immediately important. U.S. EPA is currently developing new models for application to environmental problems associated with accidental spills and releases of petroleum hydrocarbons and other oil products. Multicomponent composition data, needed as input for simulation with the EPA Research Object-Oriented Oil Spill (ERO3S) model, is unavailable in the literature due to the complexity and expense of making the measurements. Environment Canada has previously developed a database on various physical and chemical properties of crude oils and petroleum products. In this cooperative project, 10 oils and refined products identified by the U.S. EPA are characterized by the oil spill research lab of Emergencies Science and Technology Division to extend the existing information in the database. Measured oil physical properties include API gravity, density, sulphur content, water content, flash point, pour point, viscosity, surface tension, adhesion, the equation for predicting evaporation, emulsion formation, and simulated boiling point distribution. The chemical composition of the oils include hydrocarbon groups, volatile organic compounds, n-alkane distribution, distribution of alkylated polyaromatic hydrocarbon (PAH) homologues and other EPA priority PAHs, biomarker concentrations. This project will provide the most complete and comprehensive database for the selected multicomponent oils to date. The new composition data will be integrated into the existing Environment Canada oil properties database. The results will be available to the public both on the world wide web and as a database on disc.

Chandrasekar, S., Sorial, G.A., and Weaver, J.W. Determining dispersant effectiveness data for a suite of environmental conditions. Presented at: International Oil Spill Conference, Vancouver, Canada, April 7-10, 2003. 4/7/2003

Contact: James W. Weaver

Abstract: Chemical dispersants are used in oil spill response operations to enhance the dispersion of oil slicks at sea as small oil droplets in the water column. To assess the impacts of dispersant usage on oil spills, US EPA is developing a simulation model called the EPA Research Object-Oriented Oil Spill (ERO3S) model (http://www.epa.gov/athens/research/projects/eros/). Due to the complexity of chemical and physical interactions among spilled oils, dispersants and the sea, an empirical approach to the interaction between the dispersant and oil slick may provide a useful or practical approach for including dispersants in a model. The main objective of this research was to create a set of empirical data on three oils and two dispersants that has the potential for use as an input to the ERO3S model. These data were intended to give an indication of the amount of dispersal of these oils under certain environmental conditions. Recently, the US EPA developed an improved dispersant testing protocol, called the baffled flask test (BFT) which was a refinement of the swirling flask test. This protocol was the basis of the experiments conducted in this study. The variations in the effectiveness of dispersants caused by changes in oil composition, dispersant type, and the environmentally related variables of temperature, oil weathering, and rotational speed of the BFT were studied. The three oils that were tested were South Louisiana Crude Oil, Alaska North Slope Crude, and Number 2 fuel oil. Two dispersants that scored effectiveness above 85% by the BFT were selected for this study. A factorial experimental design was conducted for each of the three oils for the four factors, namely, volatilization, dispersant type, temperature and flask speed. Each of the four factors was studied at three levels except for the dispersant factor where only two dispersants are considered. Statistical analysis of the experimental data was performed separately for the three oils. Analysis of variance was conducted to determine which factors, or set of factors were related to the percent effectiveness. Empirical relationships between the amount of oil dispersed and the variables studied were developed.

Weaver, J.W. EPA's on-line calculators and training course. Presented at: U.S. EPA Office of Underground Storage Tanks Annual Conference, San Francisco, CA, March 10-12, 2003. 3/12/2003

Contact: James W. Weaver

Abstract: EPA has developed a suite of on-line calculators called "OnSite" for assessing transport of environmental contaminants int the subsurface. The calculators are available on the Internet at http://www.epa.gov/athens/onsite, and are divided into four categories: Parameter Estimates, Simple Transport Models, Unit Conversions, and Scientific Demos Since their inception in 1998, the calculators have been used by State Agencies, EPA Regional Offices and private consulting firms; and there has been a steady increase in their use. The web site will be demo-ed with emphasis on the latest additions, which include estimation of biodegradation rates from field data, uncertainty in model results and State-specific chemical data for use as inputs.With tight budgets, employee turnover and high workloads, there may be little time and money for training. EPA is adapting its modeling training course "Modeling Subsurface Transport of Petroleum Hydrocarbons" for the Internet. The course is divided into self-study modules, each with a set of objectives, 15 to 20 web pages that are enhanced with graphics and on-line calculators, review, a quiz. A certificate is automatically generated when the quiz is passed. Currently completed modules focus on fate and transport of contaminants, with more to be added in the coming months.

Weaver, J.W. Risk assessment analyses using EPA's on-line site-specific transport models and field data. Presented at: 2003 Resource Conservation and Recovery Act National Meeting: Putting Resource Conservation into Resource Conservation and Recovery Act, Washington, DC, August 12-15, 2003. 8/12/2003

Contact: James W. Weaver

Abstract: EPA has developed a suite of on-line calculators and transport models to aid in risk assessment for subsurface contamination. The calculators (www.epa.gov/athens/onsite) provide several levels of tools and data. These include tools for generating commonly-used model input parameters, transport models, unit conversions and scientific demos. Background information is provided on the calculators, along with an on-line training course on contaminant fate, transport and modeling. The purpose of these resources is to simplify and promote the correct use of the underlying ideas. An example of an input parameter calculator is the retardation factor used in subsurface transport models. The web site includes chemical data sets from superfund, regional RCRA programs and State Agencies. Thus access is provided to a suite of data sets in addition to implementing the formula itself. The available models address recharge-driven plume diving of contaminant plumes; risk estimates of contaminants at receptor locations; and the range of uncertainty in model outputs. Visitors to the web site have used these to design monitoring networks and assess the quality of modeling reports submitted in support of natural attenuation remedies. The presentation will be based on an example application of the web calculators that was drawn from a State Agency case file, and includes evaluation of field data, model application and parameter uncertainty. Suggestions for additions to the calculator site are welcome as we wish to expand the applicability of the web site by addressing more classes of problems.

Weaver, J.W., and Boufadel, M.C. Modeling dispersant interactions with oil spills. Presented at: 225th American Chemical Society National Meeting, New Orleans, LA, March 23-27, 2003. 3/23/2003

Contact: James W. Weaver

Abstract: EPA is developing a model called the EPA Research Object-Oriented Oil Spill Model (ERO3S) and associated databases to simulate the impacts of dispersants on oil slicks. Because there are features of oil slicks that align naturally with major concepts of object-oriented programming, this approach was chosen to implement the model. The two most obvious of these are the splitting of slicks into patches and the dispersal of oil into droplets. These have aspects of inheritance and polymorphism as individual slicks and droplets share some common behaviors (polymorphism) and share composition at the time of separation (inheritance). Other aspects of the object-oriented approach give the ability of the model to specify components of the graphical user interface and solution technique. This allows the computer code to contain models based upon varying conceptualization and/or suites of test problems. Each of these can have its own interface and selection of numerical solver that are generated automatically. When selected, each model can "tell" the interface what inputs are needed from the user, what numerical technique to use, and what outputs to display. The main model within ERO3S treats spreading of oil as a function of density, viscosity, interfacial tension, wind and current speeds. By imposing the implicit function theorem on the spreading equation, each of these parameters of the oil slick can vary with time. Thus change in physical properties driven by compositional change can be incorporated into the model. Compositional change is driven by primarily volatilization, but also dissolution. The data that drives the simulations is taken from four sources: chemical properties from the EPA/University of Georgia chemical property estimator called SPARC (SPARC--Performs Automated Reasoning in Chemistry), historical climate data from NOAA buoy data, a database of oil compositions and physical properties developed by Environment Canada, and a set of data on the effects of dispersants on oil slicks developed at the University of Cincinnati. The dispersant data were measured using a newly developed dispersant effectiveness testing protocol. This empirical data set includes the effects of oil composition, dispersant type, weathering, wave energy, temperature, and salinity. These properties are then matched to simulated conditions within the model. Temperature variation, for example, is treated by choosing a sequence of diurnal variations in temperature from the buoy database, generating temperature-dependent Henry's constants and solubilities from SPARC, and using the empirical dispersant data set to approximate dispersal of the oil slick. Given the time since spilling the oil, the simulated amount of weathering and the salinity, the transfer of oil into the water column due the dispersal of the oil is determined by the model. Simulation results with site-specific data from a tidal marsh in New York are presented as illustrative of planning exercises on dispersant usage.

Weaver, J.W. Models as a component of decision-making at Brownfield sites. Presented at: RevTech Conference, Pittsburg, PA, July 22-24, 2003. 7/22/2003

Contact: James W. Weaver

Abstract:

Weaver, J.W., Haas, J.E., and Small, M.C. Using subsurface transport research to achieve agency outcomes. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

Contact: James W. Weaver

Abstract: Gasoline leaks from underground storage tanks can cause ground water contamination because there are a number of organic chemicals in gasoline. These chemicals have varying properties that influence how far contamination extends from the release. Research on transport of these chemicals has provided direct input to Agency decision-making or support for program implementation. Four examples of the influence of this work will be given. In 1998, EPA convened a blue-ribbon panel to investigate all aspects of Methyl tert-butyl ether (MTBE) usage as a gasoline additive. Research done in collaboration with the New York State Department of Environmental Conservation (NYSDEC) provided the panel with detailed data on MTBE transport from sites on Long Island, which is one area of the country with significant impacts to ground water from leaking tank sites. In a later assessment of MTBE usage, the Agency pondered the question of reducing MTBE content in gasoline from 11% to 3%. A transport analysis, that used ORD developed models concluded that concentrations in ground water would indeed be reduced in proportion to the reduction in MTBE content in gasoline, but that the extent of contamination would be reduced by a much smaller amount. A company had an idea for a suite of unique tracers to be used in tank testing, but the environmental impacts of these chemicals were unknown. ORD provided an analysis of how the tracers would behave during leaks, by performing a comparative analysis MTBE and benzene transport. This allowed the Agency to make a decision on the use of the tracers with information on how these tracers would impact ground water and other environmental media (air).The most publicized application of this research to fuel problems is the OnSite on-line calculator web site at www.epa.gov/athens/onsite. The calculators were developed for State Agency regulators and private sector consultants and include practical, and sometimes simple, calculations, models and unit conversions. The site also conveys research results that can improve practice in this field. Examples where this is known to have occurred are with recharge-driven diving of plumes, effective solubility of chemicals in mixtures and input parameter-induced model uncertainty.

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Weaver, J.W. LUST On-line calculator introduction. Presented at: RevTech Conference, Pittsburg, PA, July 22--24, 2003. 7/24/2003

Contact: James W. Weaver

Abstract: EPA has developed a suite of on-line calculators to assist in performing site assessment and modeling calculations for leaking underground storage tank sites (http://www.epa.gov/athens/onsite). The calculators are divided into four types: parameter estimation, models, scientific demos and unit conversions. Parameter estimation calculators are used to estimate gradients, chemical parameters, retardation factors, multiphase partitioning and effective solubilities. Simple models are included to perform transport analyses which include transport of contaminants to receptors, diving of plumes due to recharge, and estimates of uncertainty in model outcomes. Scientific demos illustrate concepts concerning subsurface flow and transport, including for example the effects of borehole dilution on observed concentrations. Unit conversions for parameters unique to this field (hydraulic conductivity, Henry's law constants, rate constants) are included as aids to correct site assessment and analysis. Since their beginning in 1999, the calculators have proven to be a useful tool as evidenced by steady increase in their usage. EPA is currently adapting the calculators to address a wider variety of problems by including parameter values for more chemicals and by developing a model for chlorinated solvent transport and transformation.

Weaver, J.W. LUST On-line calculator introduction. Presented at: RevTech Conference, Pittsburg, PA, July 22-24, 2003. 7/24/2003

Contact: James W. Weaver

Abstract:

Weaver, J.W. Models as a component of decision-making at Brownfields sites. Presented at: RevTech Conference, Pittsburg, PA, July 22-24, 2003. 7/22/2003

Contact: James W. Weaver

Abstract: Models have become an integral part of decision-making for many LUST and Brownfields sites if only because they form the basis of RCBA tiered assessments. Models, though, are based on a series of assumptions concerning how chemicals behave in the environment, how water flows through the ground, even how a contaminant release occurs. How can you identify these assumptions? We'll present a field guide to models that helps identify model assumptions and their impacts on model results. Data is important, too, and we'll show how the amount and quality of available data affect model results. In practice, inputs to models are selected from various sources, including measurements, literature, defaults, estimates, and calibration. A number of these issues are addressed by a set of on-line calculators that EPA developed for assessment of contaminated sites (www.epa.gov/athens/onsite). We'll look at calculators that can be used to estimate parameters, convert units, and assess uncertainties in calculations. Lastly we'll look at ways to evaluate modeling work. Some steps of evaluation of models can be boiled down to nearly a recipe; also needed are knowledge of fate and transport, modeling in general, and the specific details of the model used.

Weaver, J.W. Risk assessment analyses using EPA's on-line site-specific transport models and field data. Presented at: 2003 Resource Conservation and Recovery Act National Meeting: Putting Resource Conservation into Resource Conservation and Recovery Act, Washington, DC, August 12-15, 2003. 8/13/2003

Contact: James W. Weaver

Abstract:

Presented *Published*

Hilal, S.H., Carreira, L.A., and Karickhoff, S.W. Estimation of physiochemical properties of organic compounds by SPARC. Presented at: 225th American Chemical Society National Meeting, New Orleans, LA, March 23-27, 2003. 3/23/2003

Contact: Said H. Hilal

Abstract: The computer program SPARC (SPARC Performs Automated Reasoning in Chemistry) has been under development for several years to estimate physical properties and chemical reactivity parameters of organic compounds strictly from molecular structure. SPARC uses computational algorithms based on fundamental chemical structure theory to estimate a variety of reactivity parameters. Resonance models were developed/calibrated on more than 5000 light absorption spectra, whereas electrostatic interaction models were developed using more than 4500 ionization pKas in water. Solvation models (i.e., dispersion, induction, etc) have been developed using more than 8000 physical property data points on properties such as vapor pressure, boiling point, solubility, Henry's constant, GC retention times, Kow, etc. At the present time, SPARC predicts ionization pKa, carboxylic acid ester hydrolysis rate constant, E1/2 reduction potential in many solvents, gas phase electron affinity and numerous physical properties for a broad range of molecular structures.

Johnston, J.M., Hoff, D., Hoogerheide, R., Edgar, R., Wall, D., and Ducheneaux, C. Mercury contamination of subsistence fisheries on Tribal lands: A partnership of ORD, Region 8 and Cheyenne River Sioux Reservation. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

Contact: John M. Johnston

Abstract: In a prior collaborative 3 year study with the Cheyenne River Sioux Tribe Department of Environmental Protection (CRST DEP), and the Agencies' Environmental Response Team, RegionVIII investigated Hg levels in fish tissues from the Cheyenne River and Lake Oahe in South Dakota. In 2000, the CRST released a fish advisory recommending less consumption of fish, especially for sensitive individuals within their population (pregnant and elderly). One mitigating risk management recommendation from the CRST to its constituents was to consume fish from livestock ponds, which, having no influence from mining related activities and at the time, presumably would have lower concentrations of mercury in fish tissue. However, fish from livestock ponds with seemingly similar outward appearances had significant differences in accumulation in both the same species or within species of the same trophic position.The goals of the ongoing RARE project involving the Ecosystems Research Division (ORD/NERL) are twofold: 1) Determine the source and dominant pathways of methyl mercury bioaccumulation in fish tissue (presumably due to aerial deposition and/or naturally occurring sources), and 2) Make risk management recommendations to tribal members to reduce mercury exposures. The goal here is to use the results from the first objective to make future fish stocking recommendations in ponds with the least potential for bioaccumulation of methyl mercury. Sampling of biotic and environmental media during the characterization phase will be used to support the application of the USEPA Watershed Characterization System (WCS) and Mercury Cycling Model (MCM) models. USEPA and Tribal personnel completed an initial comprehensive sampling effort in the Summer of 2002. Mercury was detected in soil samples across the region, and high levels of methyl mercury were found in aquatic invertebrates, e.g., caddisflies (110 ppb), copepods (810ppb). Region VIII personnel have developed and installed a low-budget atmospheric deposition sampler on site to characterize the source term of loadings to the ponds and surrounding watersheds. Initial results confirm high levels of methyl mercury in aquatic food webs, with communities dominated by predatory zooplankton to be much more contaminated than ponds dominated by herbivorous plankton (Cladocerans). Smaller ponds appear to be at greater risk for greater methyl mercury bioaccumulation. Sample collection is ongoing in support of model development to fully characterize the fate and transport of mercury and its biomagnification in these managed aquatic ecosystems of the Sioux Tribe.

Johnston, J.M., Hoff, D., Hoogerheide, R., Edgar, R., Wall, D., and Ducheneaux, C. Mercury risk management in livestock ponds on the Cheyenne River Sioux Reservation. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

Contact: John M. Johnston

Abstract: In a prior collaborative 3 year study with the Cheyenne River Sioux Tribe Department of Environmental Protection (CRST DEP), and the Agencies' Environmental Response Team, RegionVIII investigated Hg levels in fish tissues from the Cheyenne River and Lake Oahe in South Dakota. In 2000, the CRST released a fish advisory recommending less consumption of fish, especially for sensitive individuals within their population (pregnant and elderly). One mitigating risk management recommendation from the CRST to its constituents was to consume fish from livestock ponds, which, having no influence from mining related activities and at the time, presumably would have lower concentrations of mercury in fish tissue. However, fish from livestock ponds with seemingly similar outward appearances had significant differences in accumulation in both the same species or within species of the same trophic position.The goals of the ongoing RARE project involving the Ecosystems Research Division (ORD/NERL) are twofold: 1) Determine the source and dominant pathways of methyl mercury bioaccumulation in fish tissue (presumably due to aerial deposition and/or naturally occurring sources), and 2) Make risk management recommendations to tribal members to reduce mercury exposures. The goal here is to use the results from the first objective to make future fish stocking recommendations in ponds with the least potential for bioaccumulation of methyl mercury. Sampling of biotic and environmental media during the characterization phase will be used to support the application of the USEPA Watershed Characterization System (WCS) and Mercury Cycling Model (MCM) models. USEPA and Tribal personnel completed an initial comprehensive sampling effort in the Summer of 2002. Mercury was detected in soil samples across the region, and high levels of methyl mercury were found in aquatic invertebrates, e.g., caddisflies (110 ppb), copepods (810ppb). Region VIII personnel have developed and installed a low-budget atmospheric deposition sampler on site to characterize the source term of loadings to the ponds and surrounding watersheds. Initial results confirm high levels of methyl mercury in aquatic food webs, with communities dominated by predatory zooplankton to be much more contaminated than ponds dominated by herbivorous plankton (Cladocerans). Smaller ponds appear to be at greater risk for greater methyl mercury bioaccumulation. Sample collection is ongoing in support of model development to fully characterize the fate and transport of mercury and its biomagnification in these managed aquatic ecosystems of the Sioux Tribe.

Kraemer, S.R. Preventing contamination of public water supply wells using computerized modeling and mapping tools. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

Contact: Stephen R. Kraemer

Abstract: The EPA Office of Research and Development and the Office of Ground Water and Drinking Water have collaborated since 1998 on the development of a public domain ground-water flow modeling system designed to facilitate capture zone delineation and protection area mapping for public water supply wells in the United States. This activity is authorized by the Safe Drinking Water Act, and implemented through the state and tribe Wellhead Protection Programs (WHPP) and Source Water Assessment Planning (SWAP). The 32-bit windows software, called WhAEM2000, provides an interactive computer environment for the delineation of protection areas based on radius methods, well in uniform-flow solutions, and geohydrologic modeling methods. Protection areas are designed with and overlaid upon US Geological Survey Digital Line Graph (DLG) or other electronic base maps. Base maps for the country and the WhAEM2000 software are available for download from the EPA Center for Exposure Assessment Modeling web site. Geohydrologic modeling for steady pumping wells, including the influence of hydrological boundaries, such as rivers, recharge, no-flow boundaries, and inhomogeneity zones, is accomplished using the state-of-the-art numerical modeling technique known as the analytic element method. Reverse gradient tracelines of known residence time emanating from the pumping center are used to delineate the capture zones. WhAEM2000 has on-line help and tutorials, and good modeling practice documentation. A "Working with WhAEM2000" case study is available for the wellfield of Vincennes, Indiana, which is located in the glacial outwash of the Wabash River. The software development team includes Haitjema Consulting, LLC (Bloomington, IN), Computer Sciences Corp (Athens), and WHPA Inc (Bloomington, IN). It is anticipated that managing the potential for leaks and spills of contaminants in the properly delineated source water protection zone will result in better water quality at the faucet for millions of Americans.

Kraemer, S.R. Preventing contamination of public water supply wells using computerized modeling and mapping tools. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

Contact: Stephen R. Kraemer

Abstract: The EPA Office of Research and Development and the Office of Ground Water and Drinking Water have collaborated since 1998 on the development of a public domain ground-water flow modeling system designed to facilitate capture zone delineation and protection area mapping for public water supply wells in the United States. This activity is authorized by the Safe Drinking Water Act, and implemented through the state and tribe Wellhead Protection Programs (WHPP) and Source Water Assessment Planning (SWAP). The 32-bit windows software, called WhAEM2000, provides an interactive computer environment for the delineation of protection areas based on radius methods, well in uniform-flow solutions, and geohydrologic modeling methods. Protection areas are designed with and overlaid upon US Geological Survey Digital Line Graph (DLG) or other electronic base maps. Base maps for the country and the WhAEM2000 software are available for download from the EPA Center for Exposure Assessment Modeling web site. Geohydrologic modeling for steady pumping wells, including the influence of hydrological boundaries, such as rivers, recharge, no-flow boundaries, and inhomogeneity zones, is accomplished using the state-of-the-art numerical modeling technique known as the analytic element method. Reverse gradient tracelines of known residence time emanating from the pumping center are used to delineate the capture zones. WhAEM2000 has on-line help and tutorials, and good modeling practice documentation. A "Working with WhAEM2000" case study is available for the wellfield of Vincennes, Indiana, which is located in the glacial outwash of the Wabash River. The software development team includes Haitjema Consulting, LLC (Bloomington, IN), Computer Sciences Corp (Athens), and WHPA Inc (Bloomington, IN). It is anticipated that managing the potential for leaks and spills of contaminants in the properly delineated source water protection zone will result in better water quality at the faucet for millions of Americans.

Hayter, E.J. Development of modeling protocols for use in determining sediment TMDLs. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

Contact: Earl J. Hayter

Abstract: Modeling protocols for use in determining sediment TMDLs are being developed to provide the Office of Water, Regions and the States with assistance in determining TMDLs for sediment impaired water bodies. These protocols will supplement the protocols developed by the Office of Water (U.S. EPA 1999) for determining sediment TMDLs. Specifically, the modeling protocols will provide additional guidance in determining sediment TMDLs for cases where a numerical model must be used to simulate sediment transport and fate to quantify the impacts of proposed BMPs, etc. in reducing the detrimental effects of clean sediments on the impaired body of water. These protocols will describe the following: criteria for deciding when a sediment transport model should be used in developing a sediment TMDL; criteria for choosing the appropriate sediment transport and fate model to use for a given impaired water body; procedures to use for performing both model calibration and confirmation; data requirements for the recommended model; and recommended procedures for collecting/measuring the required data. Also included in the modeling protocols will be the testing of new sediment transport and fate models using an extensive data set collected on a 12-mile reach of the Housatonic River in western Massachusetts. The new models to be tested are EFDC-1D, GSTARS2c, CSED-2D (ver. 2.0), and EFDC. The modeling protocols along with the new sediment transport and fate models (and the supporting documentation and post-processors) will be given to the Office of Water for review and distribution to the Regions and States. It is anticipated that the results from this research will be useful to the Office of Water, the Regions and States in evaluating the effectiveness of proposed BMPs in reducing the detrimental impact of clean sediments on the nation's streams, rivers, lakes, reservoirs, and estuaries.

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Senter, J., Bird, S.L., and Rashleigh, B. Landscape-level indicators in small Georgia watersheds. Presented at: Georgia Water Resources Conference, Athens, GA, April 23-24, 2003. 4/23/2003

Contact: Brenda Rashleigh

Abstract: Landscape level indicators in small watersheds can be used as a screening tool to guide in-situ monitoring to confirm stream condition problems, aid listing of impaired waters under Section 303(d) of the Clean Water Act and total maximum daily load (TMDL) development, and provide reliable scientific information to energize sound local planning and land-use decisions. A series of landscape watershed indicators are developed for 12-digit HUCs in Georgia Piedmont. These landscape indicators are then compared to in-stream measures of water quality and biotic integrity at 180 different sampling sites. Indicators evaluated include impervious area, percent land cover types (forested, agricultural, developed), riparian stream cover, and point source discharges. While landscape indicators point to many in-stream quality issues, a substantial number are not indicated by these approaches.

Rashleigh, B., and Kennen, J.G. Beyond the indices: relations of habitat and fish characteristics in the Georgia Piedmont. Presented at: Georgia Water Resources Conference, Athens, GA, April 23-24, 2003. 4/23/2003

Contact: Brenda Rashleigh

Abstract: The Georgia Department of Natural Resources has conducted biological sampling at 180 stream sites in the Georgia Piedmont (1998-99) and recorded several trophic and abundance characteristics of the fish assemblages and habitat at each site. These characteristics were combined to form an index that provides a screening tool for multiple sites across the Piedmont. In this analysis we focus at the level of the individual characteristics to gain additional insight about ecological variability and the dominant environmental gradients across sites sampled. Data were stratified to control for variation associated with basin area, which resulted in a subset of 88 sites that ranged in size from 8 to 39 km2. Principal Components Analysis (PCA) indicated that important patterns in fish data were related to the number of benthic invertivore, cyprinid, and simple lithophilic species; and pioneering vs. sunfish species. In addition, PCA indicated that habitat variability was related to riffle amount, sediment deposition and embeddedness, and bank stability, and stream width and depth. Multiple regression indicated that the number of benthic invertivore, cyprinid, and lithophilic species appeared to be primarily associated with substrate characteristics. These results can be used to guide protection and management activities in the Georgia Piedmont, and support restoration efforts of impaired streams in the state.

Rashleigh, B., and Randall, D.J. Modeling the response of fish populations to eutrophication. Presented at: Ecological Society of America Annual Meeting, Savannah, GA, August 3-8, 2003. 8/3/2003

Contact: Brenda Rashleigh

Abstract: Eutrophication resulting from nonpoint source pollution is one of the largest environmental problems in lakes and reservoirs around the world. Two characteristics of eutrophication, decreased dissolved oxygen and increased concentration of ammonia, are known to affect fishes, yet models of eutrophication rarely include fishes. We developed a model to quantify population-level effects of eutrophication on fish. The model uses oxygen, ammonia, pH, and temperature outputs from a water quality model as driving variables and incorporates results from individual-level fish toxicology studies of growth, survival, and reproduction conducted in the laboratory. The model is applied to Lake Peipsi in Estonia/Russia. We focus on two common, commercially-important fish species, smelt (prey) and pikeperch (predator). Results indicate that the two fish species respond similarly to eutrophication, the fish populations are most sensitive to changes in oxygen, and over time, ammonia and oxygen changes are synergistic in their effects on populations. This model can be used to assess the response of the fisheries to future water quality scenarios and restoration activities.

Rashleigh, B., and Randall, D.J. Modeling the effects of eutrophication of fish populations. Presented at: Ecological Society of America Annual Meeting, Savannah, GA, August 3-8, 2003. 8/4/2003

Contact: Brenda Rashleigh

Abstract:

Rashleigh, B. Stream fish habitat suitability and the risk of population decline. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

Contact: Brenda Rashleigh

Abstract: Over half of the streams in the Mid-Atlantic Highlands have fish communities that are in fair or poor condition, and the EPA concluded that physical habitat alteration represents the greatest potential stressor across this region. A quantitative method for relating habitat quality to biological endpoints is needed in order for managers and researchers to understand the link between this stressor and fish community condition. Here, a model of fish habitat suitability that was developed by the U.S. Fish and Wildlife Service is applied in this region. Longnose dace is used as an indicator species for the most sensitive component of the fish community. Habitat suitability for longnose dace is determined by stream depth, temperature, substrate type, and natural cover and shelter. Available stream data are used to calculate an overall measure of habitat suitability. The measure of habitat suitability is then incorporated into a stage-structured population dynamics model for longnose dace. It is assumed that habitat suitability affects the carrying capacity for fish in these streams. The longnose dace population model incorporates uncertainty to provide estimates of population size through time. The outcome of this work is a modeling tool that can forecast the risk of fish population decline, in response to habitat alteration, over various time frames. The general result from this work is important because it provides managers with a method to quantitatively incorporate biological endpoints into decision-making for TMDLs. Specific results for the Mid-Atlantic Highlands can allow managers, in particular the Canaan Valley Institute, an EPA partner, to evaluate the response of biological endpoints to stream management alternatives and restoration scenarios for streams of this region.

Rashleigh, B. Population decline in stream fish. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

Contact: Brenda Rashleigh

Abstract: Over half of the streams in the Mid-Atlantic Highlands have fish communities that are in fair or poor condition, and the EPA concluded that physical habitat alteration represents the greatest potential stressor across this region. A quantitative method for relating habitat quality to biological endpoints is needed in order for managers and researchers to understand the link between this stressor and fish community condition. Here, a model of fish habitat suitability that was developed by the U.S. Fish and Wildlife Service is applied in this region. Longnose dace is used as an indicator species for the most sensitive component of the fish community. Habitat suitability for longnose dace is determined by stream depth, temperature, substrate type, and natural cover and shelter. Available stream data are used to calculate an overall measure of habitat suitability. The measure of habitat suitability is then incorporated into a stage-structured population dynamics model for longnose dace. It is assumed that habitat suitability affects the carrying capacity for fish in these streams. The longnose dace population model incorporates uncertainty to provide estimates of population size through time. The outcome of this work is a modeling tool that can forecast the risk of fish population decline, in response to habitat alteration, over various time frames. The general result from this work is important because it provides managers with a method to quantitatively incorporate biological endpoints into decision-making for TMDLs. Specific results for the Mid-Atlantic Highlands can allow managers, in particular the Canaan Valley Institute, an EPA partner, to evaluate the response of biological endpoints to stream management alternatives and restoration scenarios for streams of this region.

Washington, J.W. Nutrients in watersheds: developing enhanced modeling tools. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

Contact: John W. Washington

Abstract: Nutrient enrichment is one of the most important stressors causing water-resource impairment. These impairments are causing devastating changes: 1) high nitrate concentrations have rendered the groundwaters and reservoirs in many regions impotable -- especially in the rural areas of the US heartland where these sources are important domestic-water sources; 2) eutrophic effects in many fresh surface waters are stimulating harmful species -- e.g., the zebra mussel in the Great Lakes and pfiesteria in the Neuse River; and 3) the commercial productivity of our nation's coastal waters is in the midst of protracted decline, e.g. hypoxia and "dead zones" in estuaries of the Gulf of Mexico. Because of these and other effects, unchecked nutrient fluxes in the environment constitute one of the gravest impacts on the quality of life in the US. This project is divided into two major areas: 1) Process Science; and 2) Model Development. The Process Science research aims to identify and better elucidate specific sources of uncertainty with respect to nutrient fate in the environment. In the Modeling Development research area, several models are being developed in parallel. We plan to use some of these models to illuminate relations among media that we intend to quantify as we understand them better, e.g., effect of groundwater nutrients on surface-water quality. We plan to link other models in an open architecture environment that will be available to Program-Office users, e.g., Sediment Diagenesis and WASP. This improved suite of models is being developed in partnerships with Region 4, Office of Water (OW) National Nutrient Criteria Program (NNCP), USDA/ARS; and USGS.

Washington, J.W., Burke, Jr., R.A., Ambrose, Jr., R.B., Hayter, E.J., Kraemer, S.R., Stevens, C.T., and Zepp, R.G. Nutrients in watersheds: developing enhanced modeling tools. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

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Babendreier, J.E. National-scale multimedia risk assessment for hazardous waste disposal. Presented at: International Workshop on Uncertainty, Sensitivity, and Parameter Estimation for Multimedia Environmental Modeling, Rockville, MD, August 19-21, 2003. 8/19/2003

Contact: Justin E. Babendreier

Abstract:

Poeter, E., Babendreier, J.E., Hill, M., Doherty, J., and Banta, E.R. JUPITER Project - merging inverse problem formulation technologies. Presented at: International Workshop on Uncertainty, Sensitivity, and Parameter Estimation for Multimedia Environmental Modeling, Rockville, MD, August 19-21, 2003. 8/19/2003

Contact: Justin E. Babendreier

Abstract: The JUPITER (Joint Universal Parameter IdenTification and Evaluation of Reliability) project seeks to enhance and build on the technology and momentum behind two of the most popular sensitivity analysis, data assessment, calibration, and uncertainty analysis programs used in environmental applications: PEST (Doherty, 1994, 2002) and UCODE (Poeter and Hill, 1998). These programs are universal in that they can be applied to any computer model; both have very flexible methods for interacting with application models through ASCII files. PEST and UCODE have enjoyed substantial success. Their future, however, depends on their transition into a well-designed, flexible Application Programming Interface (API) that will support new ways of interacting with application models and new, sophisticated capabilities. Much of the technology incorporated in UCODE and PEST has been investigated thoroughly enough that its strengths, weaknesses, and advantageous uses are fairly well known. The frontier of model calibration and associated analysis methods includes pursuits that will benefit from a stable, modularly programmed, full-featured, well-designed, thoroughly documented foundation. JUPITER will provide that foundation for the PEST and UCODE developers, the work of our contemporaries and, we hope, the work of coming generations

Jan 1, 2003 - Dec 31, 2003

Presented Published

Castleton, K., Babendreier, J.E., Fine, S., Banta, E.R., Hill, M., Markstrom, S., and Leavesley, G. An overview of the uncertainty analysis, sensitivity analysis, and parameter estimation (UA/SA/PE) API and how to implement it. Presented at: International Workshop on Uncertainty, Sensitivity, and Parameter Estimation for Multimedia Environmental Modeling, Rockville, MD, August 19-21, 2003. 8/19/2003

Contact: Justin E. Babendreier

Abstract: The Application Programming Interface (API) for Uncertainty Analysis, Sensitivity Analysis, andParameter Estimation (UA/SA/PE API) (also known as Calibration, Optimization and Sensitivity and Uncertainty (CUSO)) was developed in a joint effort between several members of both the Framework Software Workgroup and the Uncertainty and Parameter Estimation Workgroup of the Federal Interagency Steering Committee on Multimedia Environmental Modeling (ISCMEM). The primary purpose for its undertaking, the development of the current draft UA/SA/PE API presented here today attempts to initiate discussion and increase cooperation among the various Federal Agencies in moving towards a common software programming approach for the future development of sharable tools and methods for conducting uncertainty analysis, sensitivity analysis, and parameter estimation.

Babendreier, J.E., Parmar, R.S., Wolfe, K., Uter, S., and McKendrick, M. PC-based supercomputing for uncertainty and sensitivity analysis of models. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

Contact: Justin E. Babendreier

Abstract: Evaluating uncertainty and sensitivity of multimedia environmental models that integrate assessments of air, soil, sediments, groundwater, and surface water is a difficult task. It can be an enormous undertaking even for simple, single-medium models (i.e. groundwater only) described by only a handful of variables and a unique set of site-specific data. The challenge then of examining ever more complex multimedia models, with 100's to 1000's of variables, is a formidable one. Today, quantitative assessment of integrated multimedia models that simulate hundreds of sites, spanning multiple geographical and ecological regions is becoming a standard risk assessment question for national policy development.A characteristic of uncertainty and sensitivity analyses for very high order models (VHOMs - indicating large numbers of variables) is their need for significant levels of computational capacity to perform large numbers of individual model simulations. While this aspect is emerging as a critical area for environmental model evaluation, resources for Windows-based, PC-based modeling have been limited by an associated lack of supercomputing capacity. Supercomputing achieved through use of personal computer (PC) clusters has expanded rapidly in recent years. Less common though are clusters that support Windows-based approaches. To facilitate model evaluation tasks for EPA's modeling systems, NERL-Athens has developed a Windows-based 270+ GHz PC-based Supercomputer for Model Uncertainty and Sensitivity Evaluation (SuperMUSE). Design and construction of SuperMUSE is described here. Extendable to many of EPA's computer models, conceptual layout of an accompanying platform-independent, Java-based parallel processing software tool set is also discussed. Together, the hardware and software tool set concept represents a key component of future modeling frameworks that the Agency is moving towards, and will ultimately strengthen our ability to validate regulatory-based modeling efforts. Advantages of the technology developed include: 1) the approach is scalable to individual user (or program office) needs (i.e. clustering from 2 to 2000 PCs), 2) it can be applied to any Windows-based modeling system (and also works for Linux systems), 3) its targeted to deliver a specific capability (i.e. uncertainty and sensitivity analyses), 4) it's a local solution, delivering to researchers and clients autonomy from large supercomputing centers formally providing these services, and 5) it's cheap and can be constructed and operated by relative novices with limited knowledge of computer science. Relating this to how we meet client needs, examples of national-scale and site-scale multimedia application are presented for key environmental exposure and risk assessment problems.

Babendreier, J.E., Parmar, R.S., Wolfe, K., Uter, S., and McKendrick, M. PC-based supercomputing for uncertainty and sensitivity analysis of models. Presented at: Science Forum 2003, Washington, DC, May 5-7, 2003. 5/5/2003

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Babendreier, J.E. Uncertainty and sensitivity analyses for integrated human health and ecological risk assessment of hazardous waste disposal. Presented at: 2003 Resource Conservation and Recovery Act National Meeting: Putting Resource Conservation into Resource Conservation and Recovery Act, Washington, DC, August 12-15, 2003. 8/13/2003

Contact: Justin E. Babendreier

Abstract: While there is a high potential for exposure of humans and ecosystems to chemicals released from hazardous waste sites, the degree to which this potential is realized is often uncertain. Conceptually divided among parameter, model, and modeler uncertainties imparted during simulation, inaccuracy in model predictions result principally from lack of knowledge and data. In comparison, sensitivity analysis can lead to a better understanding of how models respond to variation in their inputs, which in turn can be used to better focus laboratory and field-based data collection efforts on processes and parameters that contribute most to uncertainty in outputs. Evaluating uncertainty and sensitivity in environmental models can be a difficult task, even for low-order, single-medium constructs driven by a unique set of site-specific data. Quantitative assessment of integrated, multimedia models that simulate hundreds of sites, spanning multiple geographical and ecological regions, will ultimately require a comparative approach using several techniques, coupled with sufficient computational power. Residing within the Framework for Risk Analysis in Multimedia Environmental Systems (FRAMES), the Multimedia, Multipathway, and Multireceptor Risk Assessment (3MRA) modeling system is being developed by EPA for use in assessment of hazardous waste management facilities. The 3MRA modelling system includes a set of 17 science modules that collectively simulate release, fate and transport, exposure, and risk associated with hazardous contaminants disposed of in land-based waste management units (WMU). The 3MRA model currently encompasses 922 input variables, over 185 of which are explicitly stochastic. A characteristic of uncertainty analysis (UA) and sensitivity analysis (SA) for very high order models (VHOMs) like 3MRA is their need for significant computational capacity to perform relatively redundant simulations. While UA/SA is emerging as a critical area for environmental model evaluation, Windows-based models have been limited by a lack of supercomputing capacity. Equally, higher-order UA/SA algorithms warrant investigation to determine their efficacy in establishing requisite confidence in the use of VHOMs for regulatory decision-making. Design of SuperMUSE, a 215 GHz PC-based, Windows-based Supercomputer for Model Uncertainty and Sensitivity Evaluation is described. Research is reported for an uncertainty analysis and sensitivity analysis of benzene disposal using 3MRA that describes the relative importance of various exposure pathways in driving risk levels for ecological receptors and human health, evaluating aspects of both site-scale and national scale assessments. Incorporating landfills, waste piles, aerated tanks, surface impoundments, and land application units, the site-based data used in the analysis included 201 national facilities representing 419 site-WMU combinations

Babendreier, J.E. Uncertainty and sensitivity analyses for integrated human health and ecological risk assessment of hazardous waste disposal. Presented at: 2003 Resource Conservation and Recovery Act National Meeting: Putting Resource Conservation into Resource Conservation and Recovery Act, Washington, DC, August 12-15, 2003. 8/14/2003

Contact: Justin E. Babendreier

Abstract:

Uncertainty, sensitivity, and parameter estimation in risk assessment modeling. Presented at: International Workshop on Uncertainty, Sensitivity, and Parameter Estimation for Multimedia Environmental Modeling, Rockville, MD, August 19-21, 2003. 8/19/2003

Contact: Justin E. Babendreier

Abstract:

Knightes, C., and Ambrose, Jr., R.B. Modeling mercury fate in various water bodies. Presented at: Combustion Assistance Teleconference Series, Athens, GA, August 21, 2003. 8/21/2003

Contact: Christopher D. Knightes

Abstract:

Jan 1, 2003 - Dec 31, 2003

Presented Published

JOURNAL

Bird, S.L. Book review of "Ecological Effects of Roads". Journal of Environmental Quality 32 (3):1151 (2003). EPA/600/J-03/366. 6/2/2003

Contact: Sandra L. Bird

Abstract: Throughout the world, roads have become a permanent part of our environment. The ecological effects of roads and traffic are as consequential as other topical issues such as losses in biological diversity and damage by exotic and invasive species. However, this issue has usually received less attention from environmental managers, ecologists, and the public in general. Roadways impact ecological function through a variety of mechanisms from vehicular mortality of wildlife to hydrologic alterations. The effects of roads are incremental and cascading-roads lead to more roads and other development. This book discusses the biology of roads and roadside verges, describes the effects of roads and traffic, and discusses methods for mitigating the adverse effects of roads on the environment. This book aims to be a practical guide to the general issues and solutions for the ecological impacts of roads.

Bouchard, D.C. Cosolvent effects on phenanthrene sorption-desorption on a fresh-water sediment. Environmental Toxicology and Chemistry 22 (4):736-740 (2003). EPA/600/J-03/328. 4/1/2003

Contact: Dermont Bouchard

Abstract: This study evaluated the effects of the water-miscible cosolvent methanol on the sorption-desorption of phenanthrene by the natural organic matter (NOM) of a fresh-water sediment. A biphasic pattern was observed in the relationship between the log of the carbon-normalized sorption distribution coefficient (Koc) and the volumetric fraction of methanol (fc) that was accounted for with phenanthrene solubility data. Results also indicated that methanol elicited additional effects on phenanthrene sorption beyond the solution phase effects. The level of fc was observed to have a significant effect on sorption-desorption hysteresis, with hysteresis being greater for treatments where phenanthrene and sediment were equilibrated with methanol-phenanthene solutions, but desorbed with aqueous solutions. These results are discussed in light of the deformable pore network of the rubbery-glassy NOM polymer construct.

Burke, Jr., R.A., Molina, M., Cox, J.E., Osher, L.J., and Piccolo, M.C. Stable carbon isotope ratio and composition of microbial fatty acids in tropical soils. Journal of Environmental Quality 32 (1):198-206 (2003). EPA/600/J-03/067. 1/3/2003

Contact: Roger A. Burke

Abstract: The soil microbial community plays a critical part in tropical ecosystem functioning through its role in the soil organic matter (SOM) cycle. This study evaluates the relative effects of soil type and land use on: (1) soil microbial community structure and (2) the contribution of SOM derived from the original forest vegetation to the functioning of pasture and sugarcane ecosystems. We used principal components analysis (PCA) of soil phospholipid fatty acid (PLFA) profiles to evaluate microbial community structure and PLFA stable carbon isotope ratios (d13C) as indicators of the d13C of microbial substrates. Soil type mainly determined the relative proportions of gram positive versus gram negative bacteria whereas land use primarily determined the relative proportion of fungi, protozoa, and actinomycetes versus other types of microorganisms. Application of a simple model to our PLFA d13C data from land use chronosequences indicates that forest derived SOM is actively cycled for appreciably longer times in sugarcane ecosystems developed on Andisols (mean turnover time = 50 years) than in sugarcane ecosystems developed on an Oxisol (mean turnonver time = 13 years). Our analyses indicate that soil chronosequence PLFA d13C measurements can be useful indicators of the contribution that SOM derived from the original vegetation makes to continued ecosystem function under the new land use.

Loux, N.T. An exact method for relating zwitterionic microscopic to macroscopic acidity constants. Chemical Speciation and Bioavailability 15 (2):47-51 (2003). 600/J-03/380. 7/15/2003

Contact: Nicholas T. Loux

Abstract: Zwitterions are aqueous solvated molecules simultaneously possessing one negatively and one positively charged site. Although electroneutral, the environmental interaction of zwitterions with other ionic species is likely to differ significantly from the behavior of comparable electroneutral species without charged sites. Amino acids, the zwitterionic species that have received the most historical scrutiny, are believed to possess at least four microscopic acidity constants: ka = [H+] [+H3NRCOO-]/[+H3NRCOOH], kb = [H+] [H2NRCOOH]/[+H3NRCOOH], kc = [H+] [H2NRCOO-]/[+H3NRCOO-], and kd = [H+] [H2NRCOO-]/[H2NRCOOH]. Unfortunately, due to their comparable energetics, these microscopic acidity constants cannot be discerned using standard potentiometric titration procedures. In response, experimentally observable macroscopic constants (K1 and K2) have historically been related to the microscopic constants with the following relationships: K1 = ka + kb and 1/K2 = 1/kc + kd. It will be demonstrated that these equations are approximations suitable for restricted pH ranges and that more exact expressions can be derived: K1 = ka + kb + kcka/[H+] + kdkb/[H+] and 1/K2 = 1/kd + 1/kc + [H+]/kakc + [H+]/kbkd.

Kenneke, J.F., and Weber, E.J. Reductive dehalogenation of halomethanes in iron- and sulfate-reducing sediments. 1. Reactivity pattern analysis. Environmental Science & Technology 37 (4):713-720 (2003). EPA/600/J-03/150. 2/15/2003

Contact: Eric J. Weber

Abstract: The incorporation of reductive transformations into environmental fate models requires the characterization of natural reductants in well-characterized sediments and aquifer materials. For this purpose, reactivity patterns (i.e., the range and relative order of reactivity) for a series of halogenated methanes were measured in an iron- and sulfate reducing sediment, as well as model systems representing iron sulfide and Fe(II) associated with Fe(III) containing minerals. The strong similarity in reaction patterns between the iron- and sulfate-reducing sediments suggests a common mechanism for reductive transformation. The comparison of reactivity patterns measured in the sediment and model systems, in addition to those reported for the reduction of halogenated methanes in iron porphyrin and mercaptojuglone model systems, suggests that Fe(II) adsorbed to Fe(III) containing minerals is the dominant reductant in both the iron- and sulfate-reducing sediments despite the significant formation of FeS.

Richardson, S.D. Water analysis: emerging contaminants and current issues. Analytical Chemistry 75 (12):2831-2857 (2003). EPA/600/J-03/367. 6/15/2003

Contact: Susan D. Richardson

Abstract: This review covers developments in Water Analysis over the period of 2001-2002. A few significant references that appeared between January and February 2003 are also included. Previous Water Analysis reviews have been very comprehensive; however, in 2001, Analytical Chemistry changed its approach to include only 100-200 significant references and to mainly focus on new trends. As a result, this year the review will limit its focus to new, emerging contaminants and environmental issues that are driving most of the current research. Even with this more narrow focus, only a small fraction of the quality research publications could be discussed. Thus, this review will not be comprehensive, but will highlight new areas and only discuss representative papers in the areas of focus.

Jan 1, 2003 - Dec 31, 2003

Presented Published

Sundberg, S.E., Ellington, J.J., Evans, J.J., Keys, D., and Fisher, J.W. Accumulation of perchlorate in tobacco plants: development of a plant kinetic model. Journal of Environmental Monitoring 5 (3):505-512 (2003). EPA/600/J-03/326. 5/12/2003

Contact: James J. Ellington

Abstract: Previous studies have shown that tobacco plants are tolerant of perchlorate and will accumulate perchlorate in plant tissues. This research determined the uptake, translocation, and accumulation of perchlorate in tobacco plants. Three hydroponics growth studies were completed under greenhouse conditions. Depletion of perchlorate in the hydroponics nutrient solution and accumulation of perchlorate in plant tissues were determined at two-day intervals using ion chromatography. Perchlorate primarily accumulated in tobacco leaves, yielding a substantial storage capacity for perchlorate. Mass balance results show that perchlorate degradation was negligible in plants. Tobacco plants were show to effectively accumulate perchlorate over a wide range of initial concentrations (10 ppb to 100 ppm) from the hydroponics solution. Results suggest that tobacco plants are potential plants for the phytoremediation of perchlorate. A mathematical model was developed to describe the distribution of perchlorate in tobacco plants under rapid growth conditions. The distribution of inorganic chemicals such as perchlorate has not been modeled previously. The Plant Kinetic (PK) model defined a plant as a set of compartments, described by mass balance differential equations and plant-specific physiological parameters. Data obtained from a separate hydroponics growth study with multiple solution perchlorate concentrations were used to validate predicted root, stem, and leaf concentrations. There was good agreement between model predictions and measured concentrations in the plant. The model, once adequately validated, can be applied to other terrestrial plants and inorganic chemicals currently used for both phytoremediation and ecological risk assessment.

Collette, T.W., Williams, T.L., Urbansky, E.T., Magnuson, M.L., Hebert, G.N., and Strauss, S.H. Analysis of hydroponic fertilizer matrixes for perchlorate: comparison of analytical techniques. Analyst 128 (1):88-97 (2003). EPA/600/J-02/431. 1/15/2003

Contact: Timothy W. Collette

Abstract: Seven retail hydroponic nitrate fertilizer products, two liquid and five solid, were comparatively analyzed for the perchlorate anion (ClO_4^-) by ion chromatography (IC) with suppressed conductivity detection, complexation electrospray ionization mass spectrometry (cESI-MS), normal Raman spectroscopy, and infrared spectroscopy using an attenuated total reflectance crystal (ATR-FTIR) coated with a thin film of an organometallic ion-exchange compound. Three of the five solid products were found by all techniques to contain perchlorate at the level of approximately 100-350 mg kg^{-1}. The remaining products did not contain perchlorate above the detection level of any of the techniques. Comparative analysis using several analytical techniques that depend on different properties of perchlorate allow for a high degree of certainty in both the qualitative and quantitative determinations. This proved particularly useful for these samples, due to the complexity of the matrix. Analyses of this type, including multiple spectroscopic confirmations, may also be useful for other complicated matrixes (e.g., biological samples) or in forensic/regulatory frameworks where data are likely to be challenged. While the source of perchlorate in these hydroponic products is not known, the perchlorate-to-nitrate concentration ratio (w/w) in the aqueous extracts is generally consistent with the historical weight percent of water soluble components in caliche, a nitrate-bearing ore predominantly in Chile. This ore, which is the only well-established natural source of perchlorate, is mined and used, albeit minimally, as a nitrogen source in some fertilizer products.

Pakdeesusuk, U., Jones, W.J., Lee, C.M., Garrison, A.W., O'Niell, W.L., Freedman, D.L., Coates, J.T., and Wong, C.S. Changes in enantiomeric fractions during microbial reductive dechlorination of PCB132, PCB149, and Aroclor 1254 in Lake Hartwell sediment microcosms. Environmental Science & Technology 37 (6):1100-1107 (2003). EPA/600/J-03/327. 3/15/2003

Contact: William J. Jones

Abstract: Enantioselectivity of microbial reductive dechlorination of chiral PCBs in sediments from Lake Hartwell, SC, was determined by microcosm studies and enantiomer-specific GC analysis. Sediments from two locations in the vicinity of the highest levels of PCB contamination were used as inocula. Dechlorination activity was monitored by concentration decreases in the spiked chiral PCBs and formation of dechlorination products using both achiral and chiral chromatography. Live microcosms spiked with PCB132 (234-236) exhibited dechlorination of PCB132 to PCB91 (236-24) and PCB51 (24-26). Meta-dechlorination was the dominant mechanism. Microcosms spiked with PCB149 (245-236) exhibited preferential para-dechlorination of PCB149 to PCB95 (236-25), followed by meta-dechlorination to PCB53 (25-26) and subsequently PCB19 (26-2). Dechlorination of chiral PCB132 and PCB149 was not enantioselective. In Aroclor 1254-spiked microcosms, reductive dechlorination of PCB149 also was non-enantioselective. These results suggest that dechlorinating enzymes responsible for dehalogenation of the chiral PCB132 and PCB149 congeners bind both enantiomers equally. Reductive dechlorination of PCB91 and PCB95, however, occurred in an enantioselective manner indicating that the dechlorinating enzymes for these PCBs are enantiomer-specific. The chlorine substitution pattern on the biphenyl ring appears to influence whether reductive dechlorination of chiral PCB congeners is enantioselective. Enantioselective PCB dechlorination by the microbial population of Lake Hartwell sediments occurs for select chiral PCBs; thus, certain chiral PCBs may be useful as markers for in situ reductive dechlorination. These results represent the first evidence of stereoselective reductive dechlorination of PCBs under controlled conditions.

Hilal, S.H., Karickhoff, S.W., and Carreira, L.A. Prediction of the vapor pressure, boiling point, heat of vaporization and diffusion coefficient of organic compounds. QSAR & Combinatorial Science 22 (6):565-574 (2003). 8/8/2003

Contact: Said H. Hilal

Abstract: The prototype computer program SPARC has been under development for several years to estimate physical properties and chemical reactivity parameters of organic compounds strictly from molecular structure. SPARC solute-solute physical process models have been developed and tested for vapor pressure (at any temperature), heat of vaporization (at 25C and the boiling point), diffusion coefficient (at 25C) and boiling point (at any pressure) for a relatively large number of organic molecules. The RMS deviation error of the predicted the vapor pressures, heats of vaporization (at any temperature) and boiling points (at any pressure) were close to the intralaboratory experimental errors.

Doherty, J., and Johnston, J.M. Methodologies for calibration and predictive analysis of a watershed model. Journal of the American Water Resources Association 39 (2):251-265 (2003). EPA/600/J-03/325. 4/15/2003

Contact: John M. Johnston

Abstract: The use of a fitted-parameter watershed model to address water quantity and quality management issues requires that it be calibrated under a wide range of hydrologic conditions. However, rarely does model calibration result in a unique parameter set. Parameter nonuniqueness can lead to predictive nonuniqueness. The extent of model predictive uncertainty should be investigated if management decisions are to be based on model projections. Using models built for four neighboring watersheds in the Neuse River Basin of North Carolina, the application of the automated parameter optimization software PEST in conjunction with the Hydrologic Simulation Program Fortran (HSPF) is demonstrated. Parameter nonuniqueness is illustrated, and a method is presented for calculating many different sets of parameters, all of which acceptably calibrate a watershed model. A regularization methodology is discussed in which models for similar watersheds can be calibrated simultaneously. Using this method, parameter differences between watershed models can be minimized while maintaining fit between model outputs and field observations. In recognition of the fact that parameter nonuniqueness and predictive uncertainty are inherent to the modeling process, PEST's nonlinear predictive analysis functionality is then used to explore the extent of model predictive uncertainty.

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Presented Published

RESEARCH RPT

Hilal, S.H. Prediction of chemical reactivity parameters and physical properties of organic compounds from molecular structure using SPARC. 2003. EPA/600/R-03/030. 3/19/2003

Contact: Said H. Hilal

Abstract: The computer program SPARC (SPARC Performs Automated Reasoning in Chemistry) has been under development for several years to estimate physical properties and chemical reactivity parameters of organic compounds strictly from molecular structure. SPARC uses computational algorithms based on fundamental chemical structure theory to estimate a variety of reactivity parameters. Resonance models were developed and calibrated on more than 5000 light absorption spectra, whereas electrostatic interaction models were developed using more than 4500 ionization pKas in water. Solvation models (i.e., dispersion, induction, dipole-dipole, hydrogen bonding, etc.) have been developed using more than 8000 physical property data points on properties such as vapor pressure, boiling point, solubility, Henry's constant, GC retention times, Kow, etc. At the present time, SPARC predicts ionization pKa (in the gas phase and in many organic solvents including water as function of temperature), carboxylic acid ester hydrolysis rate constants (as function of solvent and temperature), E(1/2) reduction potential (as function of solvents, pH and temperature), gas phase electron affinity and numerous physical properties for a broad range of molecular structures.

Hilal, S.H. Verification and validation of the SPARC model. 2003. EPA/600/R-03/033. 1/16/2003

Contact: Said H. Hilal

Abstract: Mathematical models for predicting the transport and fate of pollutants in the environment require reactivity parameter values--that is, the physical and chemical constants that govern reactivity. Although empirical structure-activity relationships that allow estimation of some constants have been available for many years, such relationships generally hold only within very limited families of chemicals. On the other hand, we are developing computer programs that predict chemical reactivity strictly from molecular structure for virtually all organic compounds. Our computer system called SPARC (SPARC Performs Automated Reasoning in Chemistry) uses computational algorithms based on fundamental chemical structure theory to estimate a large array of physical/chemical parameters. This report focuses on the verification and validation of the SPARC Model.

SYMPOS/CONF

Frick, W.E. Diverse models for solving contrasting outfall problems. Presented at: 4th International Exhibition and Conference on Environmental Technology, Athens, Greece, January 30-February 4, 2003. EPA/600/A-03/023. 1/30/2003

Contact: Walter E. Frick

Abstract: Mixing zone initial dilution and far-field models are useful for assuring that water quality criteria will be met when specific outfall discharge criteria are applied. Presented here is a selective review of mixing zone initial dilution models and relatively simple far-field transport models. An argument is made for the continued diversity of model development, based on the complexity of the problems addressed, theoretical and experimental uncertainty, model accessibility, and the long-term outlook for improvement.